**Table S1.** Total phenolic content (TPC), total flavonoid content (TFC), total saponin content (TSC), and biological activity in each plant part of *C. inophyllum* extracts, averaged across solvents**.**

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Parts** | | **TPC**  **(mg GAE/**  **g CE)** | | **TFC**  **(mg RU/g CE)** | | **TSC**  **(mg EE/g CE)** | | **IC50**  **DPPH**  **(mg/mL)** | | **IC50**  **ABTS(mg/mL)** | | **Zone of inhibitions (mm)** | | | | | | | | | | |
| **BC** | **SA** | **SE** | | **EC** | **ST** | | **KP** | | | **PA** |
| Flower | 0.53±0.28 b | | 1.14±0.28 c | | 3.73±1.12 c | | 0.13±0.16 c | | 0.08±0.03 c | | 14.54±0.77a | | 14.47±0.77 b | 8.55±0.42 a | 8.16±0.63 ab | | | 15.87±1.30 b | | 7.66±0.74 a | 12.83±2.51 c | | |
| Fruit | 0.37±0.27 c | | 1.11±0.32 c | | 1.71±0.50 d | | 0.25±0.19 b | | 0.11±0.07 a | | 14.30±1.43 a | | 14.66±1.20 b | 8.88±0.88 a | 7.98±0.45 b | | | 16.93±0.97 a | | 7.78±0.48 a | 17.24±1.47 a | | |
| Leaf | 0.52±0.32 b | | 1.91±0.20 a | | 3.41±1.51 c | | 0.31±0.41 a | | 0.09±0.06 b | | 11.14±1.43 b | | 8.60±0.45 d | 7.86±0.54 b | 7.78±0.48 b | | | 8.49±0.53 c | | 7.70±0.43 a | 9.08±0.65 d | | |
| Twig | 0.83±0.52 a | | 1.81±0.86 a | | 4.41±0.92 b | | 0.08±0.08 d | | 0.06±0.02 e | | 13.55±3.06 a | | 13.30±3.00 c | 8.72±0.83 a | 8.54±0.60 a | | | 15.38±3.03 b | | 6.69±0.63 b | 12.41±2.54 c | | |
| Bark | 0.91±0.68 a | | 1.37±1.30 b | | 6.91±1.25 a | | 0.07±0.06 e | | 0.07±0.01 d | | 14.69±1.96 a | | 15.91±1.90 a | 8.79±0.68 a | 8.50 ±0.46 a | | | 15.09±1.92 b | | 6.95±0.34 b | 14.45±1.56 b | | |

Data shown as mean ± SD from triplicate analyses. Values in a column with different lowercase superscripts indicate significant differences (*p* < 0.05). BC: *B. cereus*, SA: *S. aureus*, SE: *S. epidermidis*, EC: *E. coli*, ST: S. t*yphi*, KP: *K. pneumoniae*, PA*: P. aeruginosa*.

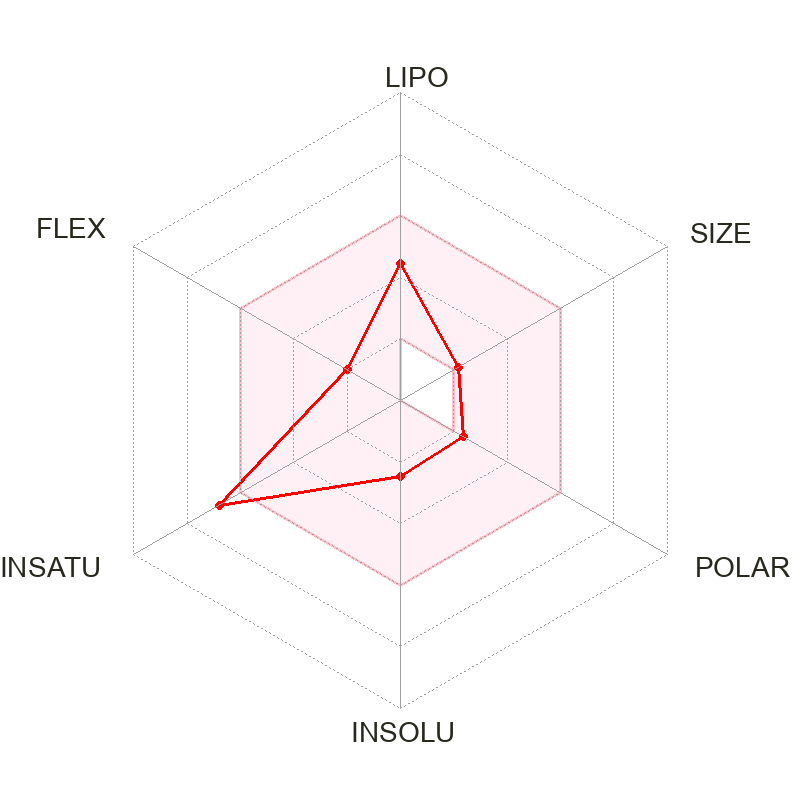
**Table S2.** Total phenolic content (TPC), total flavonoid content (TFC), total saponin content (TSC), and biological activity of *C. inophyllum* extracts, obtained from different solvents and averaged across plant parts.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Solvents** | **TPC**  **(mg GAE/**  **g CE)** | **TFC**  **(mg RU/g CE)** | **TSC**  **(mg EE/g CE)** | **IC50**  **DPPH**  **(mg/mL)** | **IC50**  **ABTS(mg/mL)** | **Zone of inhibitions (mm)** | | | | | | | | | | | | |
| **BC** | **SA** | | **SE** | | **EC** | | **ST** | | **KP** | | | **PA** |
| Hexane | 0.25±0.11 c | 1.07±0.60 c | 4.96±2.27 a | 0.40±0.27 a | 0.13±0.05 a | 15.03±2.65 a | | 14.73±3.58 a | | 8.56±0.80 ab | | 8.20±0.35 | | 15.56±3.80 a | | 7.51±0.84 | 14.51±3.75 a | |
| EtOAc | 0.68±0.16 b | 1.46±0.44 b | 3.33±1.50 b | 0.06±0.05 b | 0.06±0.01 b | 12.84±1.88 b | | 12.74±3.02 b | | 8.19±0.64 b | | 8.02±0.57 | | 13.27±3.18 c | | 7.25±0.73 | 12.20±3.29 b | |
| MeOH | 0.97±0.62 a | 1.88±0.98 a | 3.81±1.95 b | 0.04±0.04 c | 0.05±0.01 c | 13.06±1.44 b | | 12.69±2.06 b | | 8.93±0.67 a | | 8.36±0.76 | | 14.23±3.24 b | | 7.31±0.46 | 12.89±2.26 b | |

Data shown as mean ± SD from triplicate analyses. Values in a column with different lowercase superscripts indicate significant differences (*p* < 0.05). BC: *B. cereus*, SA: *S. aureus*, SE: *S. epidermidis*, EC: *E. coli*, ST: S. t*yphi*, KP: *K. pneumoniae*, PA*: P. aeruginosa*.

The bioavailability radar displays the ideal physicochemical parameters that indicate the potential of molecule compounds for oral bioavailability. The pink zone outlines the optimal range for several properties: The properties include lipophilicity (XLOGP3: -0.7 to +5.0), molecular size (MW: 150 - 500 g/mol), polarity (TPSA: 20 - 130 Å²), solubility (log S < 6), saturation (sp³ hybridization fraction of at least 0.25), and molecular flexibility (≤ 9 rotatable bonds). These parameters are used for predicting drug-likeness and guiding medicinal chemistry efforts [1].

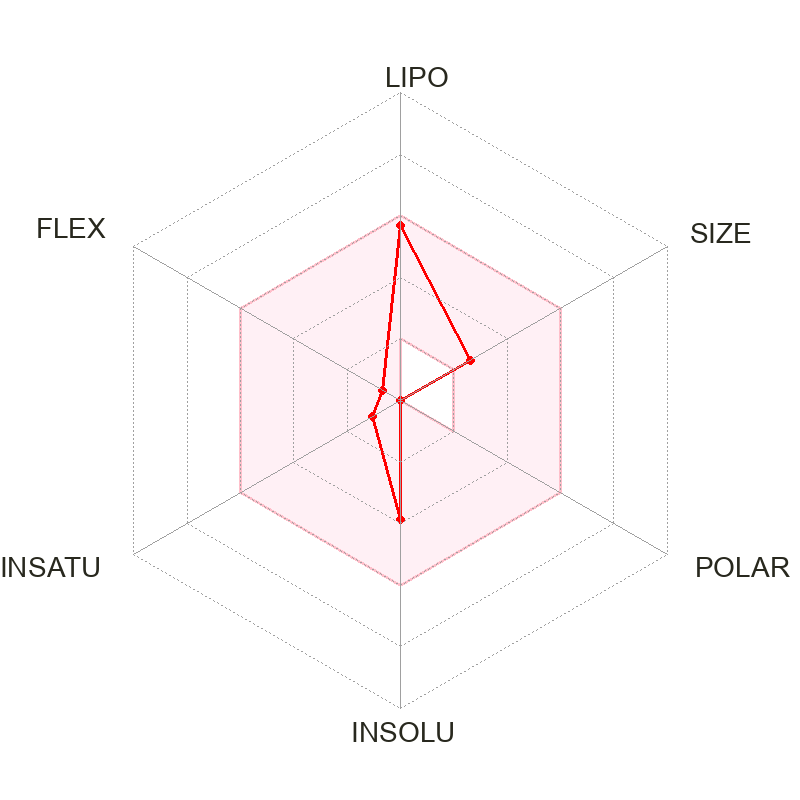
**Table S3**. SwissADME analysis of selected phytochemical compounds, identified from *C. inophyllum* flower extract.

Eugenol



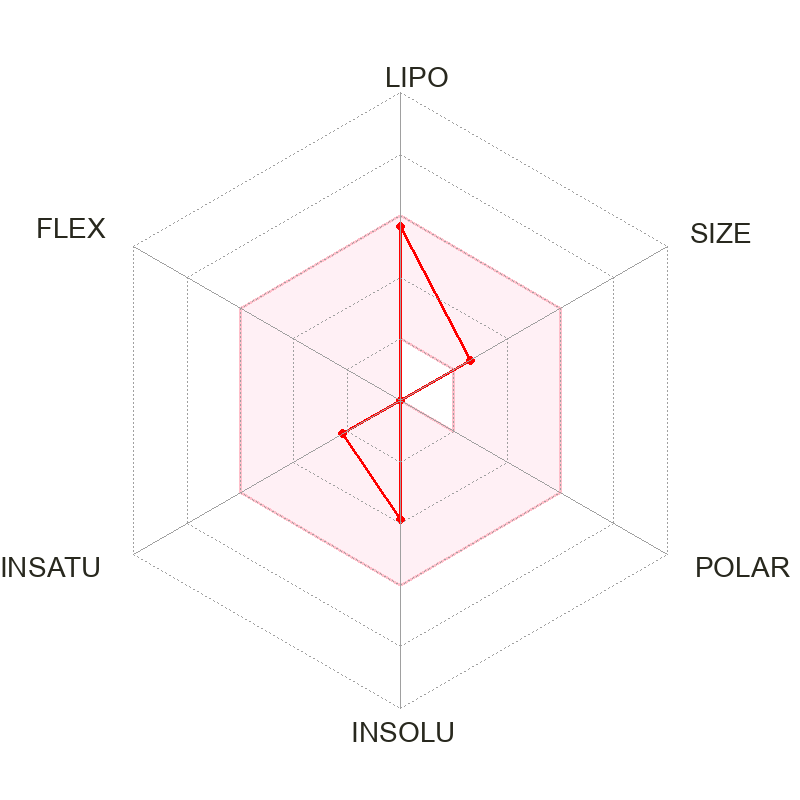
|  |  |
| --- | --- |
| SMILES | COC1=C(C=CC(=C1)CC=C)O |
| Physicochemical Properties | |
| Formula | C10H12O2 |
| Molecular weight | 164.20 g/mol |
| Num. heavy atoms | 12 |
| Num. arom. heavy atoms | 6 |
| Fraction Csp3 | 0.20 |
| Num. rotatable bonds | 3 |
| Num. H-bond acceptors | 2 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 49.06 |
| TPSA | 29.46 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 2.37 |
| Log *P*o/w (XLOGP3) | 2.27 |
| Log *P*o/w (WLOGP) | 2.13 |
| Log *P*o/w (MLOGP) | 2.01 |
| Log *P*o/w (SILICOS-IT) | 2.48 |
| Consensus Log *P*o/w | 2.25 |
| Water Solubility | |
| Log *S* (ESOL) | -2.46 |
| Solubility | 5.69e-01 mg/ml ; 3.47e-03 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -2.53 |
| Solubility | 4.90e-01 mg/ml ; 2.98e-03 mol/l |
| Class | Soluble |
| Log *S* (SILICOS-IT) | -2.79 |
| Solubility | 2.65e-01 mg/ml ; 1.61e-03 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | High |
| BBB permeant | Yes |
| P-gp substrate | No |
| CYP1A2 inhibitor | Yes |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | No |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -5.69 cm/s |
| Druglikeness | |
| Lipinski | Yes; 0 violation |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: MW<200 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 1 violation: MW<250 |
| Synthetic accessibility | 1.58 |

-Copaene



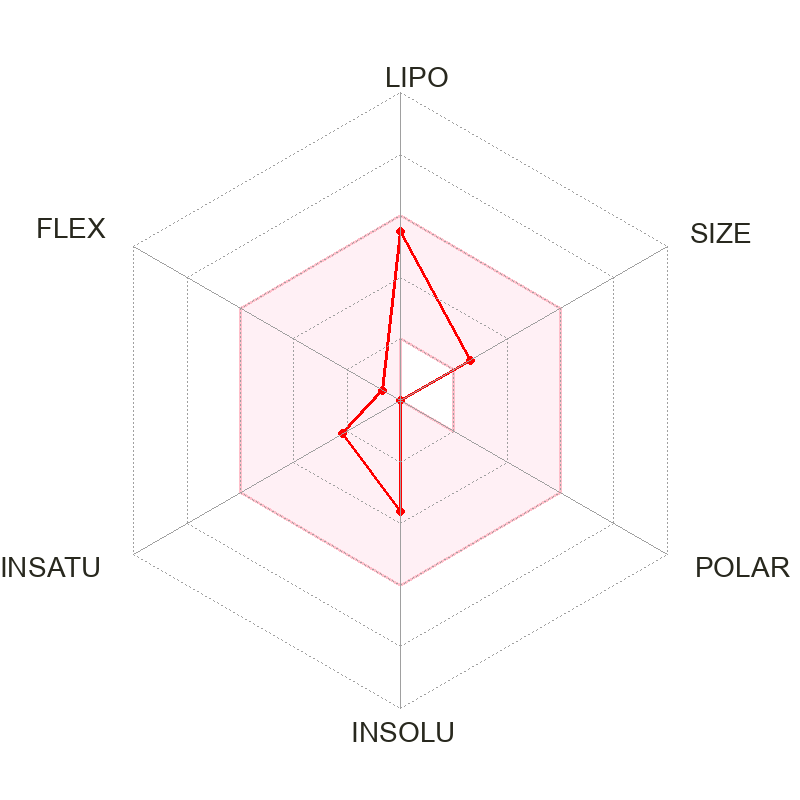


|  |  |
| --- | --- |
| SMILES | CC([C@@H]1CC[C@@]2([C@@H]3[C@H]1  [C@H]2C(=CC3)C)C)C |
| Physicochemical Properties | |
| Formula | C15H24 |
| Molecular weight | 204.35 g/mol |
| Num. heavy atoms | 15 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.87 |
| Num. rotatable bonds | 1 |
| Num. H-bond acceptors | 0 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 67.14 |
| TPSA | 0.00 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.40 |
| Log *P*o/w (XLOGP3) | 4.47 |
| Log *P*o/w (WLOGP) | 4.27 |
| Log *P*o/w (MLOGP) | 5.65 |
| Log *P*o/w (SILICOS-IT) | 3.73 |
| Consensus Log *P*o/w | 4.30 |
| Water Solubility | |
| Log *S* (ESOL) | -3.86 |
| Solubility | 2.84e-02 mg/ml ; 1.39e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -4.19 |
| Solubility | 1.32e-02 mg/ml ; 6.46e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -3.07 |
| Solubility | 1.74e-01 mg/ml ; 8.51e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | Yes |
| P-gp substrate | No |
| CYP1A2 inhibitor | Yes |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -4.37 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.62 |

-Caryophyllene



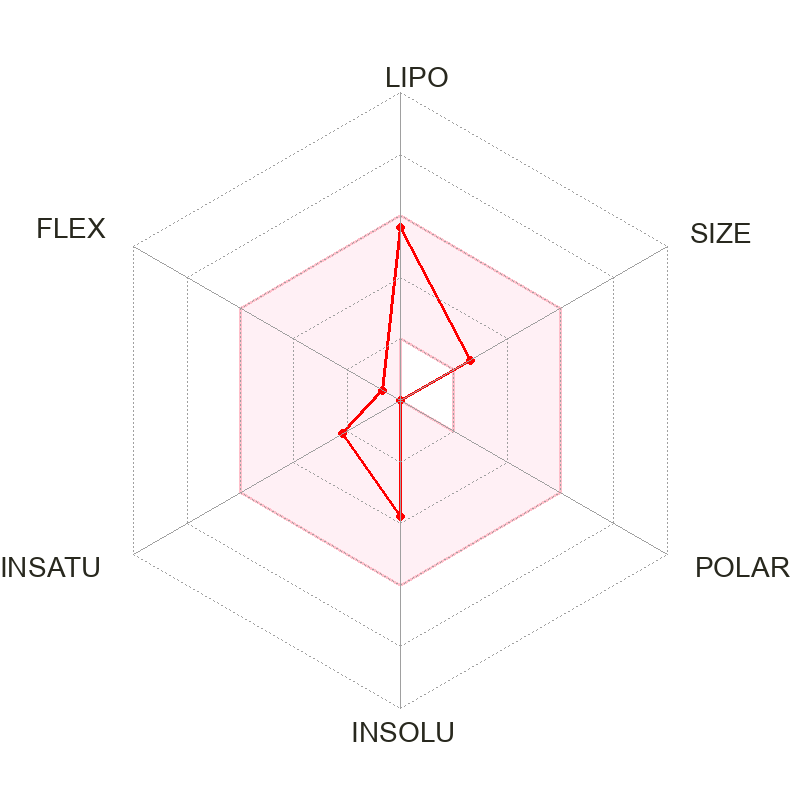
|  |  |
| --- | --- |
| SMILES | C/C/1=C\CCC(=C)[C@@H]2[C@@H](CC1)C  (C2)(C)C |
| Physicochemical Properties | |
| Formula | C15H24 |
| Molecular weight | 204.35 g/mol |
| Num. heavy atoms | 15 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.73 |
| Num. rotatable bonds | 0 |
| Num. H-bond acceptors | 0 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 68.78 |
| TPSA | 0.00 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.25 |
| Log *P*o/w (XLOGP3) | 4.38 |
| Log *P*o/w (WLOGP) | 4.73 |
| Log *P*o/w (MLOGP) | 4.63 |
| Log *P*o/w (SILICOS-IT) | 4.19 |
| Consensus Log *P*o/w | 4.24 |
| Water Solubility | |
| Log *S* (ESOL) | -3.87 |
| Solubility | 2.78e-02 mg/ml ; 1.36e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -4.10 |
| Solubility | 1.64e-02 mg/ml ; 8.01e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -3.77 |
| Solubility | 3.49e-02 mg/ml ; 1.71e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -4.44 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.51 |

-Muurolene



|  |  |
| --- | --- |
| SMILES | CC1=CC2C(CC1)C(=CCC2C(C)C)C |
| Physicochemical Properties | |
| Formula | C15H24 |
| Molecular weight | 204.35 g/mol |
| Num. heavy atoms | 15 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.73 |
| Num. rotatable bonds | 1 |
| Num. H-bond acceptors | 0 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 69.04 |
| TPSA | 0.00 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.38 |
| Log *P*o/w (XLOGP3) | 4.08 |
| Log *P*o/w (WLOGP) | 4.58 |
| Log *P*o/w (MLOGP) | 4.63 |
| Log *P*o/w (SILICOS-IT) | 3.73 |
| Consensus Log *P*o/w | 4.08 |
| Water Solubility | |
| Log *S* (ESOL) | -3.61 |
| Solubility | 5.00e-02 mg/ml ; 2.45e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -3.79 |
| Solubility | 3.35e-02 mg/ml ; 1.64e-04 mol/l |
| Class | Soluble |
| Log *S* (SILICOS-IT) | -3.07 |
| Solubility | 1.74e-01 mg/ml ; 8.51e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -4.65 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.35 |

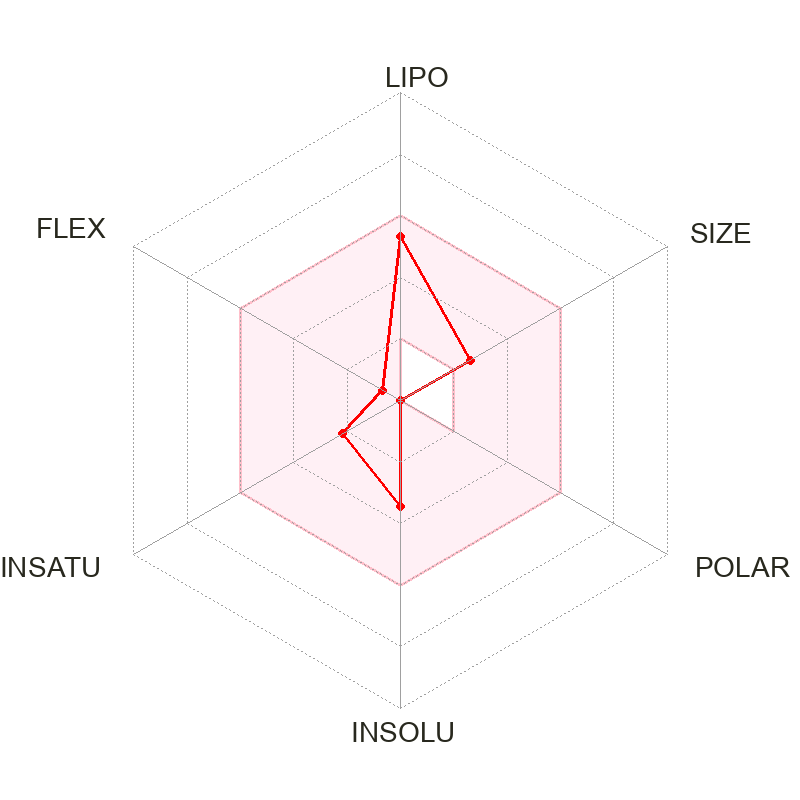
-Cadinene





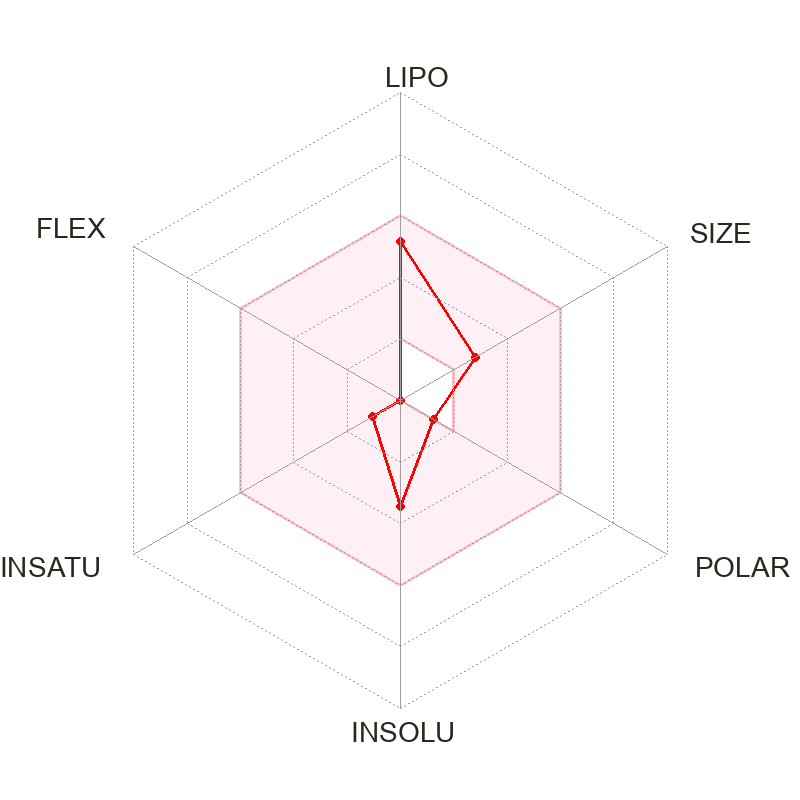
|  |  |
| --- | --- |
| SMILES | CC1=C[C@H]2[C@H](CC1)C(=C)CC[C@@H]2  C(C)C |
| Physicochemical Properties | |
| Formula | C15H24 |
| Molecular weight | 204.35 g/mol |
| Num. heavy atoms | 15 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.73 |
| Num. rotatable bonds | 1 |
| Num. H-bond acceptors | 0 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 69.04 |
| TPSA | 0.00 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.38 |
| Log *P*o/w (XLOGP3) | 4.31 |
| Log *P*o/w (WLOGP) | 4.58 |
| Log *P*o/w (MLOGP) | 4.63 |
| Log *P*o/w (SILICOS-IT) | 4.01 |
| Consensus Log *P*o/w | 4.18 |
| Water Solubility | |
| Log *S* (ESOL) | -3.76 |
| Solubility | 3.58e-02 mg/ml ; 1.75e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -4.02 |
| Solubility | 1.94e-02 mg/ml ; 9.47e-05 mol/l |
| Class | Moderately soluble |
| Log *S* (SILICOS-IT) | -3.32 |
| Solubility | 9.83e-02 mg/ml ; 4.81e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -4.49 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
|  |  |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.35 |

-Cadinene





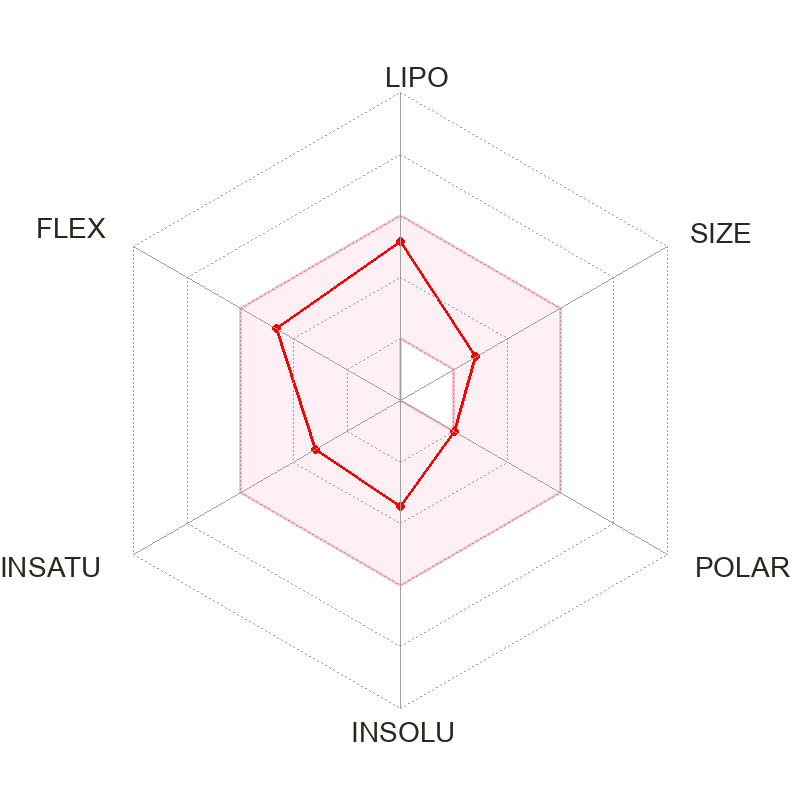
|  |  |
| --- | --- |
| SMILES | CC1=CC2C(=C(C)CCC2C(C)C)CC1 |
| Physicochemical Properties | |
| Formula | C15H24 |
| Molecular weight | 204.35 g/mol |
| Num. heavy atoms | 15 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.73 |
| Num. rotatable bonds | 1 |
| Num. H-bond acceptors | 0 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 69.04 |
| TPSA | 0.00 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.32 |
| Log *P*o/w (XLOGP3) | 3.80 |
| Log *P*o/w (WLOGP) | 4.73 |
| Log *P*o/w (MLOGP) | 4.63 |
| Log *P*o/w (SILICOS-IT) | 4.12 |
| Consensus Log *P*o/w | 4.12 |
| Water Solubility | |
| Log *S* (ESOL) | -3.43 |
| Solubility | 7.51e-02 mg/ml ; 3.67e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -3.49 |
| Solubility | 6.55e-02 mg/ml ; 3.20e-04 mol/l |
| Class | Soluble |
| Log *S* (SILICOS-IT) | -3.52 |
| Solubility | 6.19e-02 mg/ml ; 3.03e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -4.85 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
|  |  |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.14 |

Caryophyllene oxide



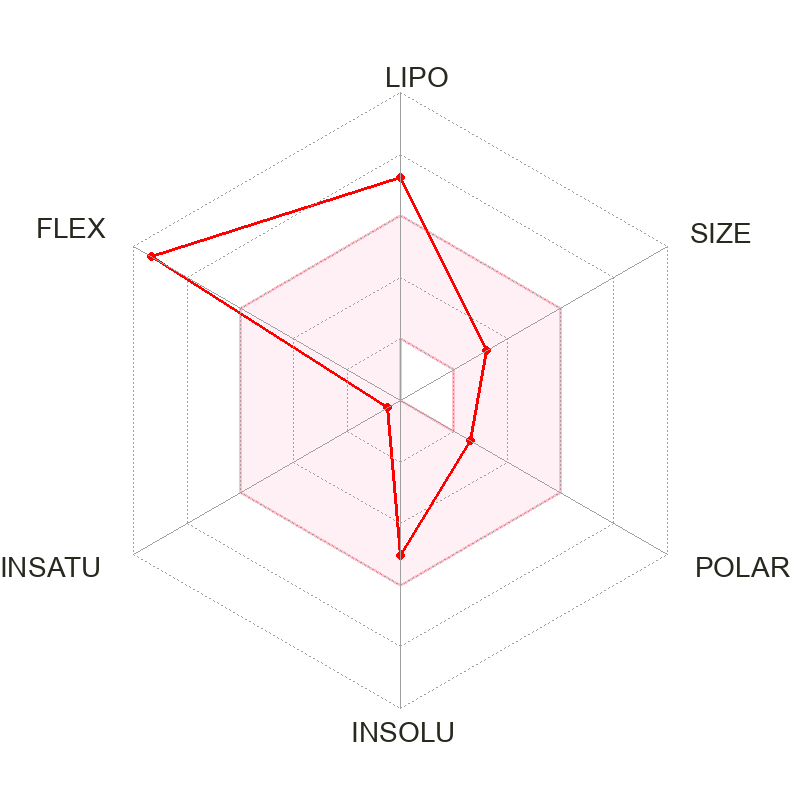
|  |  |
| --- | --- |
| SMILES | C=C1CC[C@H]2O[C@@]2(CC[C@@H]2[C@@H]1CC2(C)C)C |
| Physicochemical Properties | |
| Formula | C15H24O |
| Molecular weight | 220.35 g/mol |
| Num. heavy atoms | 16 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.87 |
| Num. rotatable bonds | 0 |
| Num. H-bond acceptors | 1 |
| Num. H-bond donors | 0 |
| Molar Refractivity | 68.27 |
| TPSA | 12.53 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.15 |
| Log *P*o/w (XLOGP3) | 3.56 |
| Log *P*o/w (WLOGP) | 3.94 |
| Log *P*o/w (MLOGP) | 3.67 |
| Log *P*o/w (SILICOS-IT) | 4.07 |
| Consensus Log *P*o/w | 3.68 |
| Water Solubility | |
| Log *S* (ESOL) | -3.45 |
| Solubility | 7.84e-02 mg/ml ; 3.56e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -3.51 |
| Solubility | 6.83e-02 mg/ml ; 3.10e-04 mol/l |
| Class | Soluble |
| Log *S* (SILICOS-IT) | -3.51 |
| Solubility | 6.81e-02 mg/ml ; 3.09e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | |
| GI absorption | High |
| BBB permeant | Yes |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -5.12 cm/s |
| Druglikeness | |
| Lipinski | Yes; 0 violation |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 2 alerts: Three-membered\_heterocycle, isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.35 |

Farnesol





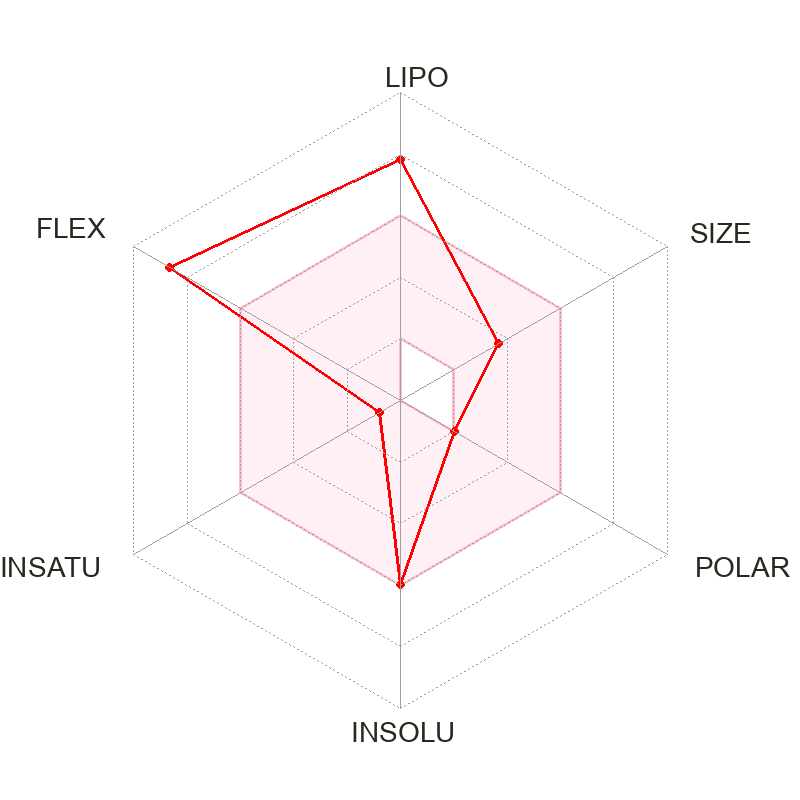
|  |  |
| --- | --- |
| SMILES | OC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C |
| Physicochemical Properties | | |
| Formula | C15H26O |
| Molecular weight | 222.37 g/mol |
| Num. heavy atoms | 16 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.60 |
| Num. rotatable bonds | 7 |
| Num. H-bond acceptors | 1 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 73.96 |
| TPSA | 20.23 Å² |
| Lipophilicity | | |
| Log *P*o/w (iLOGP) | 3.15 |
| Log *P*o/w (XLOGP3) | 3.56 |
| Log *P*o/w (WLOGP) | 4.40 |
| Log *P*o/w (MLOGP) | 3.67 |
| Log *P*o/w (SILICOS-IT) | 4.07 |
| Consensus Log *P*o/w | 3.68 |
| Water Solubility | | |
| Log *S* (ESOL) | -3.45 |
| Solubility | 7.84e-02 mg/ml ; 3.56e-04 mol/l |
| Class | Soluble |
| Log *S* (Ali) | -3.51 |
| Solubility | 6.83e-02 mg/ml ; 3.10e-04 mol/l |
| Class | Soluble |
| Log *S* (SILICOS-IT) | -3.51 |
| Solubility | 6.81e-02 mg/ml ; 3.09e-04 mol/l |
| Class | Soluble |
| Pharmacokinetics | | |
| GI absorption | High |
| BBB permeant | Yes |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | Yes |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -5.12 cm/s |
| Druglikeness | | |
| Lipinski | Yes; 0 violation |
| Ghose | Yes |
| Veber | Yes |
| Egan | Yes |
| Muegge | No; 1 violation: Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | | |
|  |  |
| PAINS | 0 alert |
| Brenk | 2 alerts: Three-membered\_heterocycle, isolated\_alkene |
| Leadlikeness | No; 2 violations: MW<250, XLOGP3>3.5 |
| Synthetic accessibility | 4.35 |

 Palmitic acid



|  |  |
| --- | --- |
| SMILES | CCCCCCCCCCCCCCCC(=O)O |
| Physicochemical Properties | |
| Formula | C16H32O2 |
| Molecular weight | 256.42 g/mol |
| Num. heavy atoms | 18 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.94 |
| Num. rotatable bonds | 14 |
| Num. H-bond acceptors | 2 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 80.80 |
| TPSA | 37.30 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 3.85 |
| Log *P*o/w (XLOGP3) | 7.17 |
| Log *P*o/w (WLOGP) | 5.55 |
| Log *P*o/w (MLOGP) | 4.19 |
| Log *P*o/w (SILICOS-IT) | 5.25 |
| Consensus Log *P*o/w | 5.20 |
| Water Solubility | |
| Log *S* (ESOL) | -5.02 |
| Solubility | 2.43e-03 mg/ml ; 9.49e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -7.77 |
| Solubility | 4.31e-06 mg/ml ; 1.68e-08 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -5.31 |
| Solubility | 1.25e-03 mg/ml ; 4.88e-06 mol/l |
| Class | Moderately soluble |
| Pharmacokinetics | |
| GI absorption | High |
| BBB permeant | Yes |
| P-gp substrate | No |
| CYP1A2 inhibitor | Yes |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -2.77 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | Yes |
| Veber | No; 1 violation: Rotors>10 |
| Egan | Yes |
| Muegge | No; 1 violation: XLOGP3>5 |
| Bioavailability Score | 0.85 |
| Medicinal Chemistry | |
|  |  |
| PAINS | 0 alert |
| Brenk | 0 alert |
| Leadlikeness | No; 2 violations: Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 2.31 |

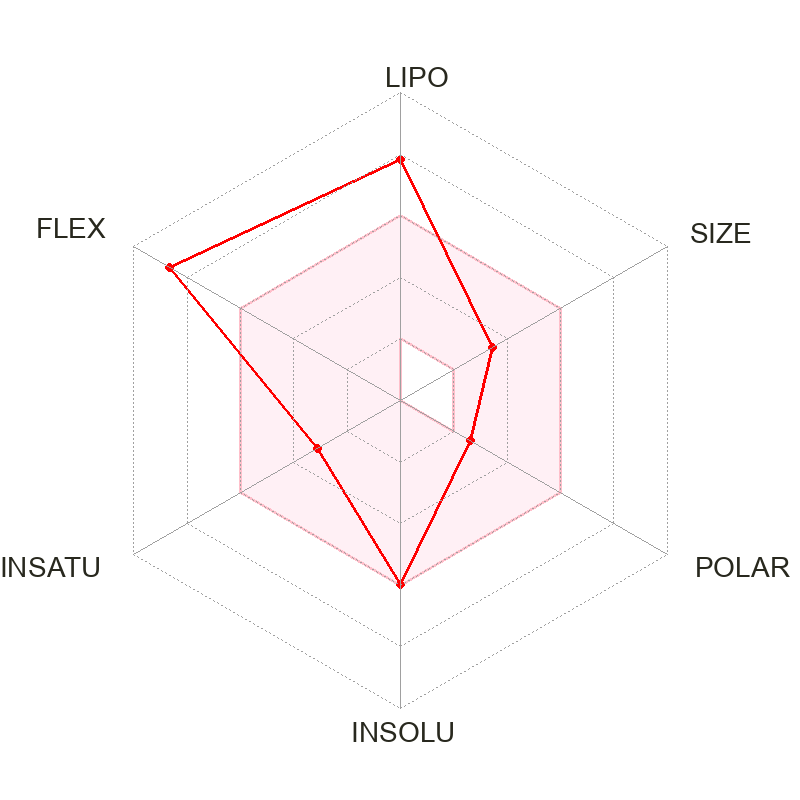
Phytol





|  |  |  |
| --- | --- | --- |
| SMILES | OC/C=C(/CCC[C@@H](CCC[C@@H](CCCC(C)  C)C)C)\C | |
| Physicochemical Properties | | |
| Formula | C20H40O | |
| Molecular weight | 296.53 g/mol | |
| Num. heavy atoms | 21 | |
| Num. arom. heavy atoms | 0 | |
| Fraction Csp3 | 0.90 | |
| Num. rotatable bonds | 13 | |
| Num. H-bond acceptors | 1 | |
| Num. H-bond donors | 1 | |
| Molar Refractivity | 98.94 | |
| TPSA | 20.23 Å² | |
| Lipophilicity | | |
| Log *P*o/w (iLOGP) | 4.85 | |
| Log *P*o/w (XLOGP3) | 8.19 | |
| Log *P*o/w (WLOGP) | 6.36 | |
| Log *P*o/w (MLOGP) | 5.25 | |
| Log *P*o/w (SILICOS-IT) | 6.57 | |
| Consensus Log *P*o/w | 6.25 | |
| Water Solubility | |
| Log *S* (ESOL) | -5.98 |
| Solubility | 3.10e-04 mg/ml ; 1.05e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -8.47 |
| Solubility | 9.94e-07 mg/ml ; 3.35e-09 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -5.51 |
| Solubility | 9.06e-04 mg/ml ; 3.05e-06 mol/l |
| Class | Moderately soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | Yes |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -2.29 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | No; 1 violation: WLOGP>5.6 |
| Veber | No; 1 violation: Rotors>10 |
| Egan | No; 1 violation: WLOGP>5.88 |
| Muegge | No; 2 violations: XLOGP3>5, Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.30 |

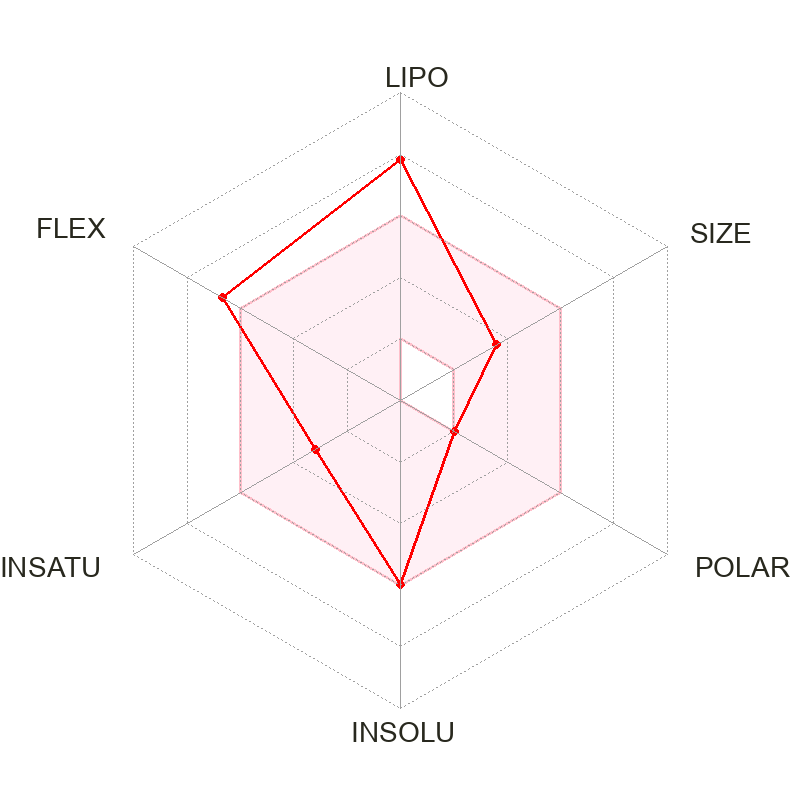
-Linolenic acid





|  |  |
| --- | --- |
| SMILES | CC/C=C\C/C=C\C/C=C\CCCCCCCC(=O)O |
| Physicochemical Properties | |
| Formula | C18H30O2 |
| Molecular weight | 278.43 g/mol |
| Num. heavy atoms | 20 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.61 |
| Num. rotatable bonds | 13 |
| Num. H-bond acceptors | 2 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 88.99 |
| TPSA | 37.30 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 4.85 |
| Log *P*o/w (XLOGP3) | 8.19 |
| Log *P*o/w (WLOGP) | 5.66 |
| Log *P*o/w (MLOGP) | 5.25 |
| Log *P*o/w (SILICOS-IT) | 6.57 |
| Consensus Log *P*o/w | 6.25 |
| Water Solubility | |
| Log *S* (ESOL) | -5.98 |
| Solubility | 3.10e-04 mg/ml ; 1.05e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -8.47 |
| Solubility | 9.94e-07 mg/ml ; 3.35e-09 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -5.51 |
| Solubility | 9.06e-04 mg/ml ; 3.05e-06 mol/l |
| Class | Moderately soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | Yes |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -2.29 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | No; 1 violation: WLOGP>5.6 |
| Veber | No; 1 violation: Rotors>10 |
| Egan | No; 1 violation: WLOGP>5.88 |
| Muegge | No; 2 violations: XLOGP3>5, Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
|  |  |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.30 |

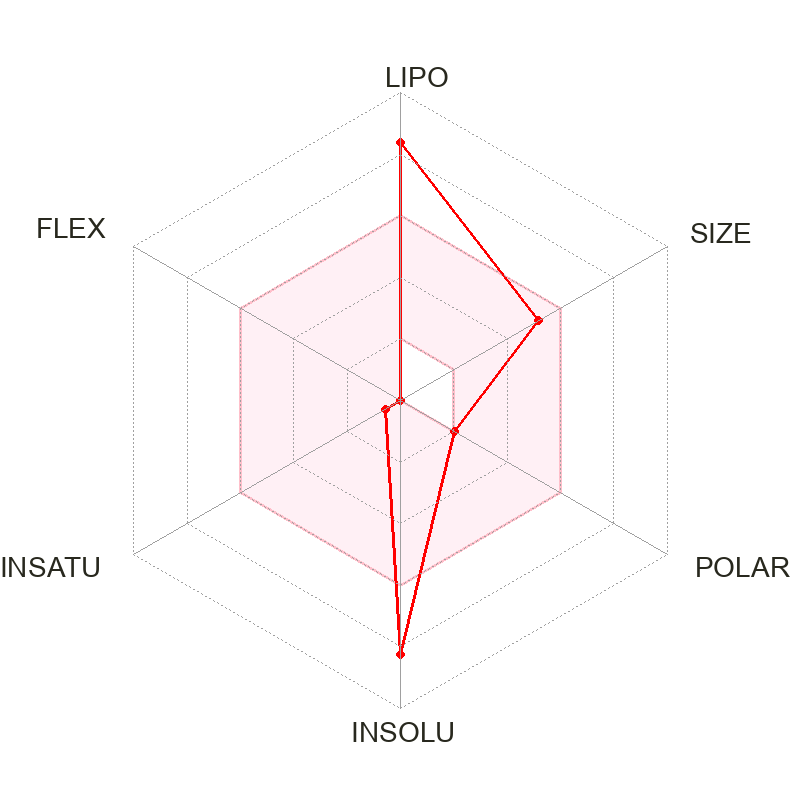
2-*cis*-Geranylgeraniol





|  |  |
| --- | --- |
| SMILES | OC/C=C(\CC/C=C(/CC/C=C(/CCC=C(C)C)\C)\C)/C |
| Physicochemical Properties | |
| Formula | C20H34O |
| Molecular weight | 290.48 g/mol |
| Num. heavy atoms | 21 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.60 |
| Num. rotatable bonds | 10 |
| Num. H-bond acceptors | 1 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 97.52 |
| TPSA | 20.23 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 4.85 |
| Log *P*o/w (XLOGP3) | 8.19 |
| Log *P*o/w (WLOGP) | 6.12 |
| Log *P*o/w (MLOGP) | 5.25 |
| Log *P*o/w (SILICOS-IT) | 6.57 |
| Consensus Log *P*o/w | 6.25 |
| Water Solubility | |
| Log *S* (ESOL) | -5.98 |
| Solubility | 3.10e-04 mg/ml ; 1.05e-06 mol/l |
| Class | Moderately soluble |
| Log *S* (Ali) | -8.47 |
| Solubility | 9.94e-07 mg/ml ; 3.35e-09 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -5.51 |
| Solubility | 9.06e-04 mg/ml ; 3.05e-06 mol/l |
| Class | Moderately soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | Yes |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | Yes |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -2.29 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | No; 1 violation: WLOGP>5.6 |
| Veber | No; 1 violation: Rotors>10 |
| Egan | No; 1 violation: WLOGP>5.88 |
| Muegge | No; 2 violations: XLOGP3>5, Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: Rotors>7, XLOGP3>3.5 |
| Synthetic accessibility | 4.30 |

[b-Amyrin](https://hmdb.ca/metabolites/HMDB0249098)





|  |  |
| --- | --- |
| SMILES | OC1CCC2(C(C1(C)C)CCC1(C2CC=C2C1(C)CCC1(C2CC(C)(C)CC1)C)C)C |
| Physicochemical Properties | |
| Formula | C30H50O |
| Molecular weight | 426.72 g/mol |
| Num. heavy atoms | 31 |
| Num. arom. heavy atoms | 0 |
| Fraction Csp3 | 0.93 |
| Num. rotatable bonds | 0 |
| Num. H-bond acceptors | 1 |
| Num. H-bond donors | 1 |
| Molar Refractivity | 134.88 |
| TPSA | 20.23 Å² |
| Lipophilicity | |
| Log *P*o/w (iLOGP) | 4.74 |
| Log *P*o/w (XLOGP3) | 9.15 |
| Log *P*o/w (WLOGP) | 8.17 |
| Log *P*o/w (MLOGP) | 6.92 |
| Log *P*o/w (SILICOS-IT) | 6.92 |
| Consensus Log *P*o/w | 7.18 |
| Water Solubility | |
| Log *S* (ESOL) | -8.25 |
| Solubility | 2.40e-06 mg/ml ; 5.62e-09 mol/l |
| Class | Poorly soluble |
| Log *S* (Ali) | -9.47 |
| Solubility | 1.44e-07 mg/ml ; 3.38e-10 mol/l |
| Class | Poorly soluble |
| Log *S* (SILICOS-IT) | -7.16 |
| Solubility | 2.93e-05 mg/ml ; 6.85e-08 mol/l |
| Class | Poorly soluble |
| Pharmacokinetics | |
| GI absorption | Low |
| BBB permeant | No |
| P-gp substrate | No |
| CYP1A2 inhibitor | No |
| CYP2C19 inhibitor | No |
| CYP2C9 inhibitor | No |
| CYP2D6 inhibitor | No |
| CYP3A4 inhibitor | No |
| Log *K*p (skin permeation) | -2.41 cm/s |
| Druglikeness | |
| Lipinski | Yes; 1 violation: MLOGP>4.15 |
| Ghose | No; 3 violations: WLOGP>5.6, MR>130, #atoms>70 |
| Veber | Yes |
| Egan | No; 1 violation: WLOGP>5.88 |
| Muegge | No; 2 violations: XLOGP3>5, Heteroatoms<2 |
| Bioavailability Score | 0.55 |
| Medicinal Chemistry | |
| PAINS | 0 alert |
| Brenk | 1 alert: isolated\_alkene |
| Leadlikeness | No; 2 violations: MW>350, XLOGP3>3.5 |
| Synthetic accessibility | 6.04 |

**REFERENCES**

1. Daina A, Michielin O, Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Rep. 2017;7(1):42717. doi: https://doi.org/10.1038/srep42717.