

germacra-1(10),4-dien-6-ol

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|-----------------------------|--|
| Inchi: | InChI=1S/C15H26O/c1-11(2)14-9-8-12(3)6-5-7-13(4)10-15(14)16/h10-11,14-16H,3,5-9H |
| InchiKey: | XETGKIFXPNGTJR-YJETWPSYSA-N |
| Formula: | C15H26O |
| SMILES: | <chem>C=C1CCCC(C)=CC(O)C(C(C)C)CC1</chem> |
| Mol. weight [g/mol]: | 222.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -22.09 | kJ/mol | Joback Method |
| hf | -370.55 | kJ/mol | Joback Method |
| hfus | 19.35 | kJ/mol | Joback Method |
| hvap | 67.20 | kJ/mol | Joback Method |
| log10ws | -4.60 | | Crippen Method |
| logp | 4.086 | | Crippen Method |
| mcvol | 208.620 | ml/mol | McGowan Method |
| pc | 1982.35 | kPa | Joback Method |
| rinsol | 1627.00 | | NIST Webbook |
| tb | 669.60 | K | Joback Method |
| tc | 875.08 | K | Joback Method |
| tf | 320.65 | K | Joback Method |
| vc | 0.758 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 598.09 | J/molxK | 669.60 | Joback Method |
| cpg | 618.60 | J/molxK | 703.85 | Joback Method |
| cpg | 637.90 | J/molxK | 738.09 | Joback Method |
| cpg | 655.97 | J/molxK | 772.34 | Joback Method |
| cpg | 672.83 | J/molxK | 806.59 | Joback Method |
| cpg | 688.46 | J/molxK | 840.83 | Joback Method |
| cpg | 702.87 | J/molxK | 875.08 | Joback Method |
| dvisc | 0.0107489 | Paxs | 320.65 | Joback Method |
| dvisc | 0.0016524 | Paxs | 378.81 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0004182 | Paxs | 436.97 | Joback Method |
| dvisc | 0.0001461 | Paxs | 495.12 | Joback Method |
| dvisc | 0.0000637 | Paxs | 553.28 | Joback Method |
| dvisc | 0.0000325 | Paxs | 611.44 | Joback Method |
| dvisc | 0.0000187 | Paxs | 669.60 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R286141&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/43-892-4/germacra-1-10-4-dien-6-ol.pdf>

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