

Germacrane-c

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| Inchi: | InChI=1S/C15H30/c1-12(2)15-10-8-13(3)6-5-7-14(4)9-11-15/h12-15H,5-11H2,1-4H3 |
| InchiKey: | IBMAYSYZAVZPY-UHFFFAOYSA-N |
| Formula: | C15H30 |
| SMILES: | CC1CCCC(C)CCC(C(C)C)CC1 |
| Mol. weight [g/mol]: | 210.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 33.61 | kJ/mol | Joback Method |
| hf | -369.21 | kJ/mol | Joback Method |
| hfus | 16.66 | kJ/mol | Joback Method |
| hvap | 49.09 | kJ/mol | Joback Method |
| log10ws | -5.03 | | Crippen Method |
| logp | 5.275 | | Crippen Method |
| mvol | 211.350 | ml/mol | McGowan Method |
| pc | 1720.31 | kPa | Joback Method |
| rinpol | 1479.00 | | NIST Webbook |
| rinpol | 1480.00 | | NIST Webbook |
| rinpol | 1482.00 | | NIST Webbook |
| ripol | 1585.00 | | NIST Webbook |
| tb | 569.45 | K | Joback Method |
| tc | 785.52 | K | Joback Method |
| tf | 228.63 | K | Joback Method |
| vc | 0.768 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 559.87 | J/molxK | 569.45 | Joback Method |
| cpg | 686.09 | J/molxK | 749.51 | Joback Method |
| cpg | 663.85 | J/molxK | 713.49 | Joback Method |
| cpg | 640.11 | J/molxK | 677.48 | Joback Method |
| cpg | 614.87 | J/molxK | 641.47 | Joback Method |
| cpg | 588.12 | J/molxK | 605.46 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 706.83 | J/molxK | 785.52 | Joback Method |
| dvisc | 0.0000798 | Paxs | 569.45 | Joback Method |
| dvisc | 0.0001235 | Paxs | 512.65 | Joback Method |
| dvisc | 0.0002130 | Paxs | 455.84 | Joback Method |
| dvisc | 0.0004291 | Paxs | 399.04 | Joback Method |
| dvisc | 0.0010907 | Paxs | 342.24 | Joback Method |
| dvisc | 0.0040194 | Paxs | 285.43 | Joback Method |
| dvisc | 0.0283190 | Paxs | 228.63 | 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=R306448&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/75-171-9/Germacrane-c.pdf>

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