

4(15)-Dehydroglobulol

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H24O/c1-9-5-6-10-12(9)13-11(14(13,2)3)7-8-15(10,4)16/h10-13,16H,1,5-8 |
| InchiKey: | GHXWXJHYNMHBGF-KBZRWBZSA-N |
| Formula: | C15H24O |
| SMILES: | <chem>C=C1CCC2C1C1C(CCC2(C)O)C1(C)C</chem> |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 115.62 | kJ/mol | Joback Method |
| hf | -245.38 | kJ/mol | Joback Method |
| hfus | 18.36 | kJ/mol | Joback Method |
| hvap | 62.68 | kJ/mol | Joback Method |
| log10ws | -3.81 | | Crippen Method |
| logp | 3.386 | | Crippen Method |
| mcvol | 191.200 | ml/mol | McGowan Method |
| pc | 2233.41 | kPa | Joback Method |
| rinpol | 1604.00 | | NIST Webbook |
| tb | 649.17 | K | Joback Method |
| tc | 856.86 | K | Joback Method |
| tf | 415.17 | K | Joback Method |
| vc | 0.727 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 575.53 | J/mol×K | 649.17 | Joback Method |
| cpg | 594.60 | J/mol×K | 683.79 | Joback Method |
| cpg | 612.82 | J/mol×K | 718.40 | Joback Method |
| cpg | 630.40 | J/mol×K | 753.02 | Joback Method |
| cpg | 647.59 | J/mol×K | 787.63 | Joback Method |
| cpg | 664.58 | J/mol×K | 822.25 | Joback Method |
| cpg | 681.62 | J/mol×K | 856.86 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R233766&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| cpg: | Ideal gas heat capacity |
| 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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