

«alpha»-Selina-11-en-4-ol

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|-----------------------------|---|
| Inchi: | InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h12-13,16H,1,5-10H |
| InchiKey: | DPQYOKVMVCQHMY-FEWQNLEASA-N |
| Formula: | C15H26O |
| SMILES: | C=C(C)C1CCC2(C)CCCC(C)(O)C2C1 |
| Mol. weight [g/mol]: | 222.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 64.59 | kJ/mol | Joback Method |
| hf | -278.76 | kJ/mol | Joback Method |
| hfus | 13.52 | kJ/mol | Joback Method |
| hvap | 62.67 | kJ/mol | Joback Method |
| log10ws | -4.39 | | Crippen Method |
| logp | 3.920 | | Crippen Method |
| mvol | 202.060 | ml/mol | McGowan Method |
| pc | 2193.84 | kPa | Joback Method |
| ripol | 2253.00 | | NIST Webbook |
| ripol | 2253.00 | | NIST Webbook |
| tb | 653.04 | K | Joback Method |
| tc | 865.92 | K | Joback Method |
| tf | 365.03 | K | Joback Method |
| vc | 0.752 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 593.33 | J/mol×K | 653.04 | Joback Method |
| cpg | 613.82 | J/mol×K | 688.52 | Joback Method |
| cpg | 633.38 | J/mol×K | 724.00 | Joback Method |
| cpg | 652.21 | J/mol×K | 759.48 | Joback Method |
| cpg | 670.53 | J/mol×K | 794.96 | Joback Method |
| cpg | 688.57 | J/mol×K | 830.44 | Joback Method |
| cpg | 706.54 | J/mol×K | 865.92 | 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=R556391&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.cheméo.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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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