

sabinene hydrate isomer

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H18O/c1-7(2)10-5-4-9(3,11)8(10)6-10/h7-8,11H,4-6H2,1-3H3/t8-,9?,10-/m |
| InchiKey: | KXSDPILWMGFJMM-RCAUJQPQSA-N |
| Formula: | C10H18O |
| SMILES: | CC(C)C12CCC(C)(O)C1C2 |
| Mol. weight [g/mol]: | 154.25 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -3.13 | kJ/mol | Joback Method |
| hf | -251.50 | kJ/mol | Joback Method |
| hfus | 6.97 | kJ/mol | Joback Method |
| hvap | 51.36 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.194 | | Crippen Method |
| mcvol | 135.910 | ml/mol | McGowan Method |
| pc | 3224.64 | kPa | Joback Method |
| ripol | 1538.00 | | NIST Webbook |
| ripol | 1538.00 | | NIST Webbook |
| ripol | 1534.00 | | NIST Webbook |
| tb | 529.23 | K | Joback Method |
| tc | 727.62 | K | Joback Method |
| tf | 327.72 | K | Joback Method |
| vc | 0.517 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 353.14 | J/molxK | 529.23 | Joback Method |
| cpg | 368.19 | J/molxK | 562.29 | Joback Method |
| cpg | 382.12 | J/molxK | 595.36 | Joback Method |
| cpg | 395.11 | J/molxK | 628.42 | Joback Method |
| cpg | 407.37 | J/molxK | 661.49 | Joback Method |
| cpg | 419.07 | J/molxK | 694.55 | Joback Method |
| cpg | 430.42 | J/molxK | 727.62 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R327876&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |

Legend

| | |
|-----------------|---|
| 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 |
| hvp: | 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 |
| ripl: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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