

trans-Sabinenehydrate

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: KXSDPILWGMGFJMM-AGROOBSYSA-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 |
| rinpol | 1100.00 | | NIST Webbook |
| rinpol | 1104.00 | | NIST Webbook |
| rinpol | 1102.00 | | NIST Webbook |
| rinpol | 1103.00 | | NIST Webbook |
| rinpol | 1087.00 | | NIST Webbook |
| rinpol | 1100.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1052.00 | | NIST Webbook |
| rinpol | 1098.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1099.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1081.00 | | NIST Webbook |
| rinpol | 1093.00 | | NIST Webbook |
| rinpol | 1096.00 | | NIST Webbook |
| rinpol | 1087.00 | | NIST Webbook |
| rinpol | 1093.00 | | NIST Webbook |
| rinpol | 1053.00 | | NIST Webbook |
| rinpol | 1097.00 | | NIST Webbook |
| rinpol | 1101.00 | | NIST Webbook |
| rinpol | 1060.00 | | NIST Webbook |

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|-------|---------|----------------------|---------------|
| ripol | 1099.00 | | NIST Webbook |
| ripol | 1474.00 | | NIST Webbook |
| ripol | 1474.00 | | NIST Webbook |
| ripol | 1474.00 | | NIST Webbook |
| ripol | 1474.00 | | NIST Webbook |
| ripol | 1438.00 | | NIST Webbook |
| tb | 529.23 | K | Joback Method |
| tc | 727.62 | K | Joback Method |
| tf | 327.72 | K | Joback Method |
| vc | 0.517 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

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

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U121973&Units=SI |

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 |

| | |
|---------------------------------------|---|
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log10 of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| m_{cvol}: | McGowan's characteristic volume |
| p_c: | Critical Pressure |
| r_{inpol}: | Non-polar retention indices |
| r_{ipol}: | Polar retention indices |
| t_b: | Normal Boiling Point Temperature |
| t_c: | Critical Temperature |
| t_f: | Normal melting (fusion) point |
| v_c: | Critical Volume |

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