

(5Z)-2,6-dimethyl-5,7-octadiene-2,3-diol

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H18O2/c1-5-8(2)6-7-9(11)10(3,4)12/h5-6,9,11-12H,1,7H2,2-4H3/b8-6- |
| InchiKey: | BTHAWHOTHGQIKC-VURMDHGXSA-N |
| Formula: | C10H18O2 |
| SMILES: | C=CC(C)=CCC(O)C(C)(C)O |
| Mol. weight [g/mol]: | 170.25 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -80.41 | kJ/mol | Joback Method |
| hf | -335.36 | kJ/mol | Joback Method |
| hfus | 16.51 | kJ/mol | Joback Method |
| hvap | 68.90 | kJ/mol | Joback Method |
| log10ws | -2.47 | | Crippen Method |
| logp | 1.641 | | Crippen Method |
| mcvol | 154.900 | ml/mol | McGowan Method |
| pc | 2865.80 | kPa | Joback Method |
| ripol | 2101.00 | | NIST Webbook |
| ripol | 2101.00 | | NIST Webbook |
| tb | 609.61 | K | Joback Method |
| tc | 785.25 | K | Joback Method |
| tf | 290.72 | K | Joback Method |
| vc | 0.579 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 403.19 | J/mol×K | 609.61 | Joback Method |
| cpg | 414.43 | J/mol×K | 638.88 | Joback Method |
| cpg | 425.05 | J/mol×K | 668.16 | Joback Method |
| cpg | 435.11 | J/mol×K | 697.43 | Joback Method |
| cpg | 444.63 | J/mol×K | 726.70 | Joback Method |
| cpg | 453.67 | J/mol×K | 755.98 | Joback Method |
| cpg | 462.25 | J/mol×K | 785.25 | 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=R334502&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 |
| 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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