

Dicyclopropylmethanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H11ClF2O2/c10-9(11,12)8(13)14-7(5-1-2-5)6-3-4-6/h5-7H,1-4H2
InchiKey: QFDFYFPPBXVDJN-UHFFFAOYSA-N
Formula: C9H11ClF2O2
SMILES: O=C(OC(C1CC1)C1CC1)C(F)(F)Cl
Mol. weight [g/mol]: 224.63

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -488.67 | kJ/mol | Joback Method |
| hf | -750.28 | kJ/mol | Joback Method |
| hfus | 17.54 | kJ/mol | Joback Method |
| hvap | 45.68 | kJ/mol | Joback Method |
| log10ws | -2.83 | | Crippen Method |
| logp | 2.550 | | Crippen Method |
| mcvol | 139.170 | ml/mol | McGowan Method |
| pc | 2841.41 | kPa | Joback Method |
| rinpola | 1168.00 | | NIST Webbook |
| rinpola | 1168.00 | | NIST Webbook |
| tb | 527.39 | K | Joback Method |
| tc | 730.20 | K | Joback Method |
| tf | 317.75 | K | Joback Method |
| vc | 0.545 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 343.31 | J/molxK | 527.39 | Joback Method |
| cpg | 357.65 | J/molxK | 561.19 | Joback Method |
| cpg | 370.93 | J/molxK | 594.99 | Joback Method |
| cpg | 383.24 | J/molxK | 628.80 | Joback Method |
| cpg | 394.64 | J/molxK | 662.60 | Joback Method |
| cpg | 405.20 | J/molxK | 696.40 | Joback Method |
| cpg | 415.01 | J/molxK | 730.20 | 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=U376251&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| 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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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