

trans-4-Methylcyclohexanol, chlorodifluoroacetate

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| Inchi: | InChI=1S/C9H13ClF2O2/c1-6-2-4-7(5-3-6)14-8(13)9(10,11)12/h6-7H,2-5H2,1H3 |
| InchiKey: | KFAUVOAPIPHBED-UHFFFAOYSA-N |
| Formula: | C9H13ClF2O2 |
| SMILES: | CC1CCC(OC(=O)C(F)(F)Cl)CC1 |
| Mol. weight [g/mol]: | 226.65 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -590.99 | kJ/mol | Joback Method |
| hf | -856.62 | kJ/mol | Joback Method |
| hfus | 17.70 | kJ/mol | Joback Method |
| hvap | 46.36 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.940 | | Crippen Method |
| mcvol | 150.030 | ml/mol | McGowan Method |
| pc | 2571.50 | kPa | Joback Method |
| rinpol | 1128.00 | | NIST Webbook |
| rinpol | 1128.00 | | NIST Webbook |
| tb | 529.23 | K | Joback Method |
| tc | 734.20 | K | Joback Method |
| tf | 300.01 | K | Joback Method |
| vc | 0.570 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 359.33 | J/molxK | 529.23 | Joback Method |
| cpg | 375.48 | J/molxK | 563.39 | Joback Method |
| cpg | 390.69 | J/molxK | 597.55 | Joback Method |
| cpg | 404.96 | J/molxK | 631.71 | Joback Method |
| cpg | 418.33 | J/molxK | 665.87 | Joback Method |
| cpg | 430.83 | J/molxK | 700.03 | Joback Method |
| cpg | 442.47 | J/molxK | 734.20 | 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=U376261&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| 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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