

Cyclohexanol, 2-methylene-3-(1-methylethenyl)-, acetate, cis-

Other names:

3-Isopropenyl-2-methylenecyclohexyl acetate, (Z)-

(Z)-2-Methylene-3-(1-methylethenyl)cyclohexyl acetate

Inchi: InChI=1S/C12H18O2/c1-8(2)11-6-5-7-12(9(11)3)14-10(4)13/h11-12H,1,3,5-7H2,2,4H3/t1

InchiKey: LJTGDIGDBFRYRO-VXGBXAGGSA-N

Formula: C12H18O2

SMILES: C=C(C)C1CCCC(OC(C)=O)C1=C

Mol. weight [g/mol]: 194.27

CAS: 54824-09-8

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -34.65 | kJ/mol | Joback Method |
| hf | -301.95 | kJ/mol | Joback Method |
| hfus | 18.78 | kJ/mol | Joback Method |
| hvap | 51.15 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.850 | | Crippen Method |
| mvol | 167.920 | ml/mol | McGowan Method |
| pc | 2298.11 | kPa | Joback Method |
| tb | 560.85 | K | Joback Method |
| tc | 769.45 | K | Joback Method |
| tf | 298.26 | K | Joback Method |
| vc | 0.629 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 414.55 | J/molxK | 560.85 | Joback Method |
| cpg | 432.66 | J/molxK | 595.62 | Joback Method |
| cpg | 449.82 | J/molxK | 630.38 | Joback Method |
| cpg | 466.06 | J/molxK | 665.15 | Joback Method |
| cpg | 481.39 | J/molxK | 699.92 | Joback Method |
| cpg | 495.80 | J/molxK | 734.69 | Joback Method |
| cpg | 509.32 | J/molxK | 769.45 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C54824098&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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