

Cyclocopacamphan-12-ol, epimer a

Inchi: InChI=1S/C15H24O/c1-8(7-16)9-4-5-14(2)10-6-11-13(12(9)10)15(11,14)3/h8-13,16H,4-7
InchiKey: TUWGUUUUJAXUPF-QAQQNOBPSA-N
Formula: C15H24O
SMILES: CC(CO)C1CCC2(C)C3CC4C(C13)C42C
Mol. weight [g/mol]: 220.35

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 169.25 | kJ/mol | Joback Method |
| hf | -237.46 | kJ/mol | Joback Method |
| hfus | 22.53 | kJ/mol | Joback Method |
| hvap | 61.35 | kJ/mol | Joback Method |
| log10ws | -3.01 | | Crippen Method |
| logp | 2.933 | | Crippen Method |
| mcvol | 184.640 | ml/mol | McGowan Method |
| pc | 2274.07 | kPa | Joback Method |
| rinpola | 1645.00 | | NIST Webbook |
| ripola | 2368.00 | | NIST Webbook |
| tb | 639.23 | K | Joback Method |
| tc | 837.50 | K | Joback Method |
| tf | 418.51 | K | Joback Method |
| vc | 0.726 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 575.79 | J/molxK | 639.23 | Joback Method |
| cpg | 593.44 | J/molxK | 672.27 | Joback Method |
| cpg | 610.25 | J/molxK | 705.32 | Joback Method |
| cpg | 626.45 | J/molxK | 738.36 | Joback Method |
| cpg | 642.30 | J/molxK | 771.41 | Joback Method |
| cpg | 658.05 | J/molxK | 804.45 | Joback Method |
| cpg | 673.93 | J/molxK | 837.50 | 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=R397850&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 |
| rinpolar: | Non-polar retention indices |
| ripolar: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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