

6,6-Dimethyl-2-methylenebicyclo[3.2.0]heptan-3-one

Inchi: InChI=1S/C10H16O/c1-6-7-5-10(2,3)8(7)4-9(6)11/h7-9,11H,1,4-5H2,2-3H3
InchiKey: USLBRUNJVYNISV-UHFFFAOYSA-N
Formula: C10H16O
SMILES: C=C1C(O)CC2C1CC2(C)C
Mol. weight [g/mol]: 152.23
CAS: 1005276-05-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 38.07 | kJ/mol | Joback Method |
| hf | -203.72 | kJ/mol | Joback Method |
| hfus | 14.60 | kJ/mol | Joback Method |
| hvap | 52.92 | kJ/mol | Joback Method |
| log10ws | -2.30 | | Crippen Method |
| logp | 1.969 | | Crippen Method |
| mcvol | 131.610 | ml/mol | McGowan Method |
| pc | 3076.16 | kPa | Joback Method |
| rinpol | 1156.90 | | NIST Webbook |
| rinpol | 1156.90 | | NIST Webbook |
| tb | 528.19 | K | Joback Method |
| tc | 723.06 | K | Joback Method |
| tf | 324.74 | K | Joback Method |
| vc | 0.500 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 335.96 | J/molxK | 528.19 | Joback Method |
| cpg | 350.83 | J/molxK | 560.67 | Joback Method |
| cpg | 364.79 | J/molxK | 593.15 | Joback Method |
| cpg | 377.93 | J/molxK | 625.63 | Joback Method |
| cpg | 390.35 | J/molxK | 658.11 | Joback Method |
| cpg | 402.17 | J/molxK | 690.59 | Joback Method |
| cpg | 413.48 | J/molxK | 723.06 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1005276050&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| h vap: | 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 |
| r in pol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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