

endo-Bicyclo[2.2.1]hept-5-en-2-carboxylic acid, 7,7-cyclopropano-2-methyl, methyl ester

Inchi: InChI=1S/C12H16O2/c1-11(10(13)14-2)7-8-3-4-9(11)12(8)5-6-12/h3-4,8-9H,5-7H2,1-2H1
InchiKey: UPOPHKONFXCKPW-YWVKMMECSA-N
Formula: C12H16O2
SMILES: COC(=O)C1(C)CC2C=CC1C21CC1
Mol. weight [g/mol]: 192.25

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 9.76 | kJ/mol | Joback Method |
| hf | -249.49 | kJ/mol | Joback Method |
| hfus | 13.72 | kJ/mol | Joback Method |
| hvap | 48.88 | kJ/mol | Joback Method |
| log10ws | -2.28 | | Crippen Method |
| logp | 2.152 | | Crippen Method |
| mvol | 150.500 | ml/mol | McGowan Method |
| pc | 2950.48 | kPa | Joback Method |
| rinpol | 1270.00 | | NIST Webbook |
| ripol | 1658.00 | | NIST Webbook |
| tb | 565.44 | K | Joback Method |
| tc | 791.70 | K | Joback Method |
| tf | 395.30 | K | Joback Method |
| vc | 0.584 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 402.36 | J/mol×K | 565.44 | Joback Method |
| cpg | 419.21 | J/mol×K | 603.15 | Joback Method |
| cpg | 434.74 | J/mol×K | 640.86 | Joback Method |
| cpg | 449.27 | J/mol×K | 678.57 | Joback Method |
| cpg | 463.09 | J/mol×K | 716.28 | Joback Method |
| cpg | 476.51 | J/mol×K | 753.99 | Joback Method |
| cpg | 489.83 | J/mol×K | 791.70 | 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=R13101&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 |
| 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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