

2-Dimethylamino-3,3-dimethylcyclo-butanecarboxylic acid

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| Inchi: | InChI=1S/C9H18N2O/c1-9(2)5-6(8(10)12)7(9)11(3)4/h6-7H,5H2,1-4H3,(H2,10,12) |
| InchiKey: | DPGXRZYPRCIJLQ-UHFFFAOYSA-N |
| Formula: | C9H18N2O |
| SMILES: | CN(C)C1C(C(N)=O)CC1(C)C |
| Mol. weight [g/mol]: | 170.25 |
| CAS: | 19244-93-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 100.95 | kJ/mol | Joback Method |
| hf | -199.15 | kJ/mol | Joback Method |
| hfus | 20.76 | kJ/mol | Joback Method |
| hvap | 53.37 | kJ/mol | Joback Method |
| log10ws | -0.89 | | Crippen Method |
| logp | 0.448 | | Crippen Method |
| mcvol | 148.340 | ml/mol | McGowan Method |
| pc | 2986.06 | kPa | Joback Method |
| tb | 546.07 | K | Joback Method |
| tc | 756.58 | K | Joback Method |
| tf | 386.69 | K | Joback Method |
| vc | 0.537 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 382.41 | J/molxK | 546.07 | Joback Method |
| cpg | 398.94 | J/molxK | 581.16 | Joback Method |
| cpg | 414.43 | J/molxK | 616.24 | Joback Method |
| cpg | 429.00 | J/molxK | 651.33 | Joback Method |
| cpg | 442.77 | J/molxK | 686.41 | Joback Method |
| cpg | 455.85 | J/molxK | 721.50 | Joback Method |
| cpg | 468.36 | J/molxK | 756.58 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.cheméo.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=C19244930&Units=SI |

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 |
| m cvol: | 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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