

Butylone, Ac

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| Inchi: | InChI=1S/C14H17NO4/c1-4-11(15(3)9(2)16)14(17)10-5-6-12-13(7-10)19-8-18-12/h5-7,1 |
| InchiKey: | IYVFCTYHZFKZDA-UHFFFAOYSA-N |
| Formula: | C14H17NO4 |
| SMILES: | CCC(C(=O)c1ccc2c(c1)OCO2)N(C)C(C)=O |
| Mol. weight [g/mol]: | 263.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -93.13 | kJ/mol | Joback Method |
| hf | -452.47 | kJ/mol | Joback Method |
| hfus | 41.00 | kJ/mol | Joback Method |
| hvap | 74.75 | kJ/mol | Joback Method |
| log10ws | -2.89 | | Crippen Method |
| logp | 1.855 | | Crippen Method |
| mvol | 198.360 | ml/mol | McGowan Method |
| pc | 2540.49 | kPa | Joback Method |
| rinpol | 2215.00 | | NIST Webbook |
| rinpol | 2215.00 | | NIST Webbook |
| tb | 741.41 | K | Joback Method |
| tc | 962.09 | K | Joback Method |
| tf | 491.65 | K | Joback Method |
| vc | 0.736 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 567.32 | J/mol×K | 741.41 | Joback Method |
| cpg | 580.97 | J/mol×K | 778.19 | Joback Method |
| cpg | 593.66 | J/mol×K | 814.97 | Joback Method |
| cpg | 605.47 | J/mol×K | 851.75 | Joback Method |
| cpg | 616.47 | J/mol×K | 888.53 | Joback Method |
| cpg | 626.75 | J/mol×K | 925.31 | Joback Method |
| cpg | 636.39 | J/mol×K | 962.09 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=R615777&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 |
| hvpap: | 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 |
| rinppl: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/117-963-3/Butylone-Ac.pdf>

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