

2-Oxetanone, 3,3-dimethyl-

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|-----------------------------|---|
| Other names: | «alpha», «alpha»-Dimethyl-«beta»-propiolactone «alpha», «alpha»-Dimethylpropiolactone Pivalic acid lactone Pivalolactone Propanoic acid, 3-hydroxy-2,2-dimethyl-, «beta»-lactone 3,3-Dimethyl-«beta»-propiolactone 3,3-Dimethyl-2-oxetanone NCI-C04126 Hydracrylic acid, 2,2-dimethyl-, «beta»-lactone Pivalic acid, hydroxy-, lactone |
| Inchi: | InChI=1S/C5H8O2/c1-5(2)3-7-4(5)6/h3H2,1-2H3 |
| InchiKey: | ULKFLOVGORAZDI-UHFFFAOYSA-N |
| Formula: | C5H8O2 |
| SMILES: | CC1(C)COC1=O |
| Mol. weight [g/mol]: | 100.12 |
| CAS: | 1955-45-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| chl | -2716.70 | kJ/mol | NIST Webbook |
| gf | -174.33 | kJ/mol | Joback Method |
| hf | -352.70 | kJ/mol | NIST Webbook |
| hfl | -395.10 | kJ/mol | NIST Webbook |
| hfus | 5.93 | kJ/mol | Joback Method |
| hvap | 42.40 | kJ/mol | NIST Webbook |
| hvap | 42.43 | kJ/mol | NIST Webbook |
| log10ws | -0.43 | | Crippen Method |
| logp | 0.569 | | Crippen Method |
| mcvol | 77.890 | ml/mol | McGowan Method |
| pc | 4615.13 | kPa | Joback Method |
| tb | 419.82 | K | Joback Method |
| tc | 640.67 | K | Joback Method |
| tf | 279.22 | K | Joback Method |
| vc | 0.290 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 156.68 | J/mol×K | 419.82 | Joback Method |
| cpg | 167.71 | J/mol×K | 456.63 | Joback Method |
| cpg | 177.94 | J/mol×K | 493.44 | Joback Method |
| cpg | 187.46 | J/mol×K | 530.25 | Joback Method |
| cpg | 196.36 | J/mol×K | 567.05 | Joback Method |
| cpg | 204.73 | J/mol×K | 603.86 | Joback Method |
| cpg | 212.66 | J/mol×K | 640.67 | 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=C1955459&Units=SI |

Legend

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|----------|---|
| chl: | Standard liquid enthalpy of combustion |
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfl: | Liquid phase 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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