

Isomethylionone

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C14H22O/c1-10-7-6-8-14(4,5)13(10)9-11(2)12(3)15/h7,9,13H,6,8H2,1-5H3/b1 |
| InchiKey: | JRJBVWJSTHECJK-PKQNBQFBNSA-N |
| Formula: | C14H22O |
| SMILES: | CC(=O)C(C)=CC1C(C)=CCCC1(C)C |
| Mol. weight [g/mol]: | 206.32 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 41.33 | kJ/mol | Joback Method |
| hf | -241.91 | kJ/mol | Joback Method |
| hfus | 19.95 | kJ/mol | Joback Method |
| hvap | 53.46 | kJ/mol | Joback Method |
| log10ws | -4.08 | | Crippen Method |
| logp | 3.904 | | Crippen Method |
| mcvol | 190.230 | ml/mol | McGowan Method |
| pc | 2058.62 | kPa | Joback Method |
| ripol | 1900.00 | | NIST Webbook |
| tb | 596.89 | K | Joback Method |
| tc | 814.96 | K | Joback Method |
| tf | 318.75 | K | Joback Method |
| vc | 0.723 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 489.05 | J/mol×K | 596.89 | Joback Method |
| cpg | 508.48 | J/mol×K | 633.24 | Joback Method |
| cpg | 526.79 | J/mol×K | 669.58 | Joback Method |
| cpg | 544.12 | J/mol×K | 705.93 | Joback Method |
| cpg | 560.60 | J/mol×K | 742.27 | Joback Method |
| cpg | 576.37 | J/mol×K | 778.62 | Joback Method |
| cpg | 591.55 | J/mol×K | 814.96 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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=R577576&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 |
| 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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/71-346-9/Isomethylionone.pdf>

Generated by Cheméo on 2024-04-26 15:19:07.15921808 +0000 UTC m=+16433996.079795392.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.