

Mintoxide

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|-----------------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C15H24O/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(16-12)13(11)15/h9,11-14H,3,5-8 |
| InchiKey: | BITBXAWCPCNKKN-XTLGRWLVSA-N |
| Formula: | C15H24O |
| SMILES: | <chem>C=C1CCC2OC1C1C(C(C)C)CCC21C</chem> |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 177.08 | kJ/mol | Joback Method |
| hf | -225.33 | kJ/mol | Joback Method |
| hfus | 23.95 | kJ/mol | Joback Method |
| hvap | 51.58 | kJ/mol | Joback Method |
| log10ws | -3.98 | | Crippen Method |
| logp | 3.792 | | Crippen Method |
| mcvol | 191.200 | ml/mol | McGowan Method |
| pc | 2027.23 | kPa | Joback Method |
| ripol | 1926.00 | | NIST Webbook |
| tb | 587.93 | K | Joback Method |
| tc | 805.89 | K | Joback Method |
| tf | 346.26 | K | Joback Method |
| vc | 0.726 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 539.56 | J/mol×K | 587.93 | Joback Method |
| cpg | 562.18 | J/mol×K | 624.26 | Joback Method |
| cpg | 583.38 | J/mol×K | 660.58 | Joback Method |
| cpg | 603.34 | J/mol×K | 696.91 | Joback Method |
| cpg | 622.22 | J/mol×K | 733.23 | Joback Method |
| cpg | 640.21 | J/mol×K | 769.56 | Joback Method |
| cpg | 657.47 | J/mol×K | 805.89 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R420074&Units=SI |
| 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 |

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 |

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<https://www.chemeo.com/cid/33-967-2/Mintoxide.pdf>

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