

Nitrous acid, cyclohexyl ester

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| Other names: | Cyclohexyl nitrite Cyclohexyl ester of nitrous acid |
| Inchi: | InChI=1S/C6H11NO2/c8-7-9-6-4-2-1-3-5-6/h6H,1-5H2 |
| InchiKey: | NRCNZCLHYWKEDX-UHFFFAOYSA-N |
| Formula: | C6H11NO2 |
| SMILES: | O=NOC1CCCCC1 |
| Mol. weight [g/mol]: | 129.16 |
| CAS: | 5156-40-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -413.26 | kJ/mol | Joback Method |
| hvap | 40.89 | kJ/mol | Joback Method |
| log10ws | -2.61 | | Crippen Method |
| logp | 2.017 | | Crippen Method |
| mcvol | 101.960 | ml/mol | McGowan Method |
| pc | 3791.65 | kPa | Joback Method |
| tb | 442.05 | K | Joback Method |
| tc | 645.77 | K | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C5156401&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

hf: Enthalpy of formation at standard conditions

| | |
|---------------------------------------|---|
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log10 of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| p_c: | Critical Pressure |
| t_b: | Normal Boiling Point Temperature |
| t_c: | Critical Temperature |

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<https://www.chemeo.com/cid/98-568-4/Nitrous-acid-cyclohexyl-ester.pdf>

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