

Cyclohexanemethyl isothiocyanate

Inchi: InChI=1S/C8H13NS/c10-7-9-6-8-4-2-1-3-5-8/h8H,1-6H2
InchiKey: RYBJNWIQNLZNPE-UHFFFAOYSA-N
Formula: C8H13NS
SMILES: S=C=NCC1CCCCC1
Mol. weight [g/mol]: 155.26
CAS: 52395-66-1

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | 129.94 | kJ/mol | Joback Method |
| hvap | 44.27 | kJ/mol | Joback Method |
| log10ws | -2.76 | | Crippen Method |
| logp | 2.670 | | Crippen Method |
| mcvol | 130.450 | ml/mol | McGowan Method |
| pc | 3231.98 | kPa | Joback Method |
| tb | 547.94 | K | Joback Method |
| tc | 798.52 | K | Joback Method |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C52395661&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

hf: Enthalpy of formation 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 |

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