

2-Tetrahydrofurfuryl isothiocyanate

Inchi: InChI=1S/C6H9NOS/c9-5-7-4-6-2-1-3-8-6/h6H,1-4H2
InchiKey: CSFIFTGMGITVRE-UHFFFAOYSA-N
Formula: C6H9NOS
SMILES: S=C=NCC1CCCO1
Mol. weight [g/mol]: 143.21
CAS: 36810-87-4

Physical Properties

Property code	Value	Unit	Source
hf	45.38	kJ/mol	Joback Method
hvap	44.16	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.268		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	524.86	K	Joback Method
tc	773.31	K	Joback Method

Sources

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=C36810874&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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