

2-Chloroethyl isothiocyanate

Inchi: InChI=1S/C3H4CINS/c4-1-2-5-3-6/h1-2H2
InchiKey: ZUWFBQUHBOUPFK-UHFFFAOYSA-N
Formula: C3H4CINS
SMILES: S=C=NCCCI
Mol. weight [g/mol]: 121.59
CAS: 6099-88-3

Physical Properties

Property code	Value	Unit	Source
hf	163.08	kJ/mol	Joback Method
hvap	37.10	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.328		Crippen Method
mcvol	83.100	ml/mol	McGowan Method
pc	4322.57	kPa	Joback Method
tb	451.42	K	Joback Method
tc	682.51	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C6099883&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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