

3-Chloropropyl isothiocyanate

Inchi: InChI=1S/C4H6CINS/c5-2-1-3-6-4-7/h1-3H2
InchiKey: ZGFOBQSQLJDLKV-UHFFFAOYSA-N
Formula: C4H6CINS
SMILES: S=C=NCCCCI
Mol. weight [g/mol]: 135.62
CAS: 2799-72-6

Physical Properties

Property code	Value	Unit	Source
hf	142.44	kJ/mol	Joback Method
hvap	39.32	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.718		Crippen Method
mcvol	97.190	ml/mol	McGowan Method
pc	3824.55	kPa	Joback Method
tb	474.30	K	Joback Method
tc	701.67	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=C2799726&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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