

Urea, 1-(2-chloroethyl)-3-methyl-3-nitroso-

Inchi: InChI=1S/C4H8CIN3O2/c1-8(7-10)4(9)6-3-2-5/h2-3H2,1H3,(H,6,9)
InchiKey: LQTIRBDBDLBOTK-UHFFFAOYSA-N
Formula: C4H8CIN3O2
SMILES: CN(N=O)C(=O)NCCCI
Mol. weight [g/mol]: 165.58
CAS: 29655-34-3

Physical Properties

Property code	Value	Unit	Source
hf	-301.40	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.548		Crippen Method
mcvol	112.540	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	508.23	K	Joback Method
tc	696.92	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C29655343&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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