

Biuret, 1-(2-chloroethyl)-5-methyl-

Inchi:	InChI=1S/C5H10CIN3O2/c1-7-4(10)9-5(11)8-3-2-6/h2-3H2,1H3,(H3,7,8,9,10,11)
InchiKey:	IQIIGIYHHDNVMK-UHFFFAOYSA-N
Formula:	C5H10CIN3O2
SMILES:	CN=C(O)NC(O)=NCCCI
Mol. weight [g/mol]:	179.60
CAS:	16813-28-8

Physical Properties

Property code	Value	Unit	Source
hf	-268.40	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.273		Crippen Method
mcvol	126.630	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	738.88	K	Joback Method
tc	936.97	K	Joback Method

Sources

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=C16813288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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