

Propanoic acid, 3-hydroxy-2[3-(2-chloroethyl)ureido]-

Inchi:	InChI=1S/C6H11CIN2O4/c7-1-2-8-6(13)9-4(3-10)5(11)12/h4,10H,1-3H2,(H,11,12)(H2,8,9)
InchiKey:	SSAHXIIXIQFLMV-UHFFFAOYSA-N
Formula:	C6H11CIN2O4
SMILES:	O=C(O)C(CO)NC(O)=NCCCI
Mol. weight [g/mol]:	210.62

Physical Properties

Property code	Value	Unit	Source
hf	-631.56	kJ/mol	Joback Method
hvap	99.56	kJ/mol	Joback Method
log10ws	0.37		Crippen Method
logp	-0.826		Crippen Method
mcvol	142.480	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	830.81	K	Joback Method
tc	1023.62	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=B6010420&Units=SI

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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