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

Inchi: InChI=1S/C6H11ClN2O4/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: C6H11ClN2O4

SMILES: O=C(O)C(CO)NC(O)=NCCCl

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010420&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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