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

Inchi: InChI=1S/C6H11Cl2N3O2/c7-1-3-9-5(12)11-6(13)10-4-2-8/h1-4H2,(H3,9,10,11,12,13)
InchiKey: YEAPZDVWWPEUCZ-UHFFFAOYSA-N
Formula: C6H11Cl2N3O2
SMILES: O=C(NCCCl)NC(=O)NCCCl
Mol. weight [g/mol]: 228.08
CAS: 16813-30-2

Physical Properties

Property code	Value	Unit	Source
gf	-13.89	kJ/mol	Joback Method
hf	-263.40	kJ/mol	Joback Method
hfus	38.18	kJ/mol	Joback Method
hvap	70.52	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	0.473		Crippen Method
mcvol	152.960	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
tb	669.79	K	Joback Method
tc	872.36	K	Joback Method
tf	475.06	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.19	J/mol×K	669.79	Joback Method
cpg	377.28	J/mol×K	703.55	Joback Method
cpg	385.77	J/mol×K	737.31	Joback Method
cpg	393.70	J/mol×K	771.08	Joback Method
cpg	401.09	J/mol×K	804.84	Joback Method
cpg	407.94	J/mol×K	838.60	Joback Method
cpg	414.30	J/mol×K	872.36	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=C16813302&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume