Urea, 1-(2-chloroethyl)-3-(3,3,5-trimethylcyclohexyl)-

Inchi: InChI=1S/C12H23ClN2O/c1-9-6-10(8-12(2,3)7-9)15-11(16)14-5-4-13/h9-10H,4-8H2,1-3H

InchiKey: DSLTZAHFAWMNRS-UHFFFAOYSA-N

Formula: C12H23ClN2O

SMILES: CC1CC(NC(=O)NCCCl)CC(C)(C)C1

Mol. weight [g/mol]: 246.78

CAS: 13908-16-2

Physical Properties

Property code	Value	Unit	Source
gf	91.63	kJ/mol	Joback Method
hf	-283.51	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	64.97	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.739		Crippen Method
mcvol	202.850	ml/mol	McGowan Method
pc	2195.89	kPa	Joback Method
tb	676.05	K	Joback Method
tc	888.41	K	Joback Method
tf	432.97	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.42	J/mol×K	676.05	Joback Method
cpg	592.53	J/mol×K	711.44	Joback Method
cpg	609.71	J/mol×K	746.84	Joback Method
cpg	626.07	J/mol×K	782.23	Joback Method
cpg	641.73	J/mol×K	817.62	Joback Method
cpg	656.78	J/mol×K	853.01	Joback Method
cpg	671.34	J/mol×K	888.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908162&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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