Urea, 1-(2-chloroethyl)-3-(3,5,7-trimethyl-1-adamantyl)-

Inchi: InChI=1S/C16H27ClN2O/c1-13-6-14(2)8-15(3,7-13)11-16(9-13,10-14)19-12(20)18-5-4-17

InchiKey: LFKQXXPDBWHTFZ-UHFFFAOYSA-N

Formula: C16H27ClN2O

SMILES: CC12CC3(C)CC(C)(C1)CC(NC(=O)NCCCl)(C2)C3

Mol. weight [g/mol]: 298.85

CAS: 33021-59-9

Physical Properties

Property code	Value	Unit	Source
gf	262.25	kJ/mol	Joback Method
hf	-142.09	kJ/mol	Joback Method
hfus	21.37	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.663		Crippen Method
mcvol	237.490	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	777.90	K	Joback Method
tc	1011.26	K	Joback Method
tf	596.91	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.87	J/mol×K	777.90	Joback Method
cpg	766.51	J/mol×K	816.79	Joback Method
cpg	789.24	J/mol×K	855.69	Joback Method
cpg	813.66	J/mol×K	894.58	Joback Method
cpg	840.33	J/mol×K	933.47	Joback Method
cpg	869.83	J/mol×K	972.37	Joback Method
cpg	902.73	J/mol×K	1011.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33021599&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