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

Inchi: InChI=1S/C16H26ClN3O2/c1-13-6-14(2)8-15(3,7-13)11-16(9-13,10-14)18-12(21)20(19-2

InchiKey: RVKXSUCLMXKRLW-UHFFFAOYSA-N

Formula: C16H26ClN3O2

SMILES: CC12CC3(C)CC(C)(C1)CC(N=C(O)N(CCCl)N=O)(C2)C3

Mol. weight [g/mol]: 327.85

CAS: 33021-99-7

Physical Properties

Property code	Value	Unit	Source
hf	-316.91	kJ/mol	Joback Method
hvap	81.81	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.262		Crippen Method
mcvol	249.040	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
tb	868.27	K	Joback Method
tc	1091.93	K	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=C33021997&Units=SI

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

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