Urea, 1-(2-chloroethyl)-3-(5,6,7,8-tetrahydro-2-naphthyl)

Inchi: InChI=1S/C13H17ClN2O/c14-7-8-15-13(17)16-12-6-5-10-3-1-2-4-11(10)9-12/h5-6,9H,1-4

InchiKey: UPQTWUWCCQECCM-UHFFFAOYSA-N

Formula: C13H17ClN2O

SMILES: O=C(NCCCl)Nc1ccc2c(c1)CCCC2

Mol. weight [g/mol]: 252.74

CAS: 13908-56-0

Physical Properties

Property code	Value	Unit	Source
gf	246.02	kJ/mol	Joback Method
hf	-32.46	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.926		Crippen Method
mcvol	193.180	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	740.80	K	Joback Method
tc	969.58	K	Joback Method
tf	491.56	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.91	J/mol×K	740.80	Joback Method
cpg	547.06	J/mol×K	778.93	Joback Method
cpg	560.18	J/mol×K	817.06	Joback Method
cpg	572.35	J/mol×K	855.19	Joback Method
cpg	583.65	J/mol×K	893.32	Joback Method
cpg	594.16	J/mol×K	931.45	Joback Method
cpg	603.97	J/mol×K	969.58	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=C13908560&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