Urea, 1-(2-chloroethyl)-3-(2-naphthyl)-

Inchi: InChI=1S/C13H13ClN2O/c14-7-8-15-13(17)16-12-6-5-10-3-1-2-4-11(10)9-12/h1-6,9H,7-8

InchiKey: BMPINTUZIXWLFQ-UHFFFAOYSA-N

Formula: C13H13ClN2O

SMILES: O=C(NCCCl)Nc1ccc2ccccc2c1

Mol. weight [g/mol]: 248.71

CAS: 13908-57-1

Physical Properties

Property code	Value	Unit	Source
gf	305.94	kJ/mol	Joback Method
hf	83.10	kJ/mol	Joback Method
hfus	36.09	kJ/mol	Joback Method
hvap	73.11	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.200		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
tb	739.12	K	Joback Method
tc	971.65	K	Joback Method
tf	493.08	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.33	J/mol×K	739.12	Joback Method
cpg	494.47	J/mol×K	777.88	Joback Method
cpg	505.67	J/mol×K	816.63	Joback Method
cpg	516.04	J/mol×K	855.39	Joback Method
cpg	525.64	J/mol×K	894.14	Joback Method
cpg	534.58	J/mol×K	932.90	Joback Method
cpg	542.94	J/mol×K	971.65	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=C13908571&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