Urea, N-(2-methylcyclohexyl)-N'-phenyl-

Other names:	1-(2-Methylcyclohexyl)-3-phenylurea
	Du Pont 1318
	Du pont herbicide 1,318
	H 1318
	N-Phenyl-N'-(2-methylcyclohexyl)urea
	NSC 131951
	Siduron
	Trey
	Tupersan
	Urea, 1-(2-methylcyclohexyl)-3-phenyl-
Inchi:	InChI=1S/C14H20N2O/c1-11-7-5-6-10-13(11)16-14(17)15-12-8-3-2-4-9-12/h2-4,8-9,11,1
InchiKey:	JXVIIQLNUPXOII-UHFFFAOYSA-N
Formula:	C14H20N2O
SMILES:	CC1CCCCC1NC(=O)Nc1ccccc1
Mol. weight [g/mol]:	232.32
CAS:	1982-49-6

Physical Properties

Property code	Value	Unit	Source
gf	246.01	kJ/mol	Joback Method
hf	-67.42	kJ/mol	Joback Method
hfus	30.76	kJ/mol	Joback Method
hvap	68.77	kJ/mol	Joback Method
log10ws	-4.11		Aqueous Solubility Prediction Method
log10ws	-4.11		Estimated Solubility Method
logp	3.387		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	715.49	K	Joback Method
tc	949.61	K	Joback Method
tf	432.35	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.69	J/mol×K	715.49	Joback Method
cpg	592.18	J/mol×K	754.51	Joback Method
cpg	609.22	J/mol×K	793.53	Joback Method
cpg	624.86	J/mol×K	832.55	Joback Method
cpg	639.16	J/mol×K	871.57	Joback Method
cpg	652.20	J/mol×K	910.59	Joback Method
cpg	664.03	J/mol×K	949.61	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1982496&Units=SI

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