Cycluron

Other names:	1,1-Dimethyl-3-cyclooctylurea
	3-Cyclooctyl-1,1-dimethylharnstoff
	3-Cyclooctyl-1,1-dimethylurea
	Cyclouron
	HS 61
	N'-Cyclooctyl-N,N-dimethylurea
	N-Cyclooctyl-N',N'-dimethylurea
	OMU
	Urea, 3-cyclooctyl-1,1-dimethyl-
	Urea, N'-cyclooctyl-N,N-dimethyl-
Inchi:	InChI=1S/C11H22N2O/c1-13(2)11(14)12-10-8-6-4-3-5-7-9-10/h10H,3-9H2,1-2H3,(H,12,1
InchiKey:	DQZCVNGCTZLGAQ-UHFFFAOYSA-N
Formula:	C11H22N2O
SMILES:	CN(C)C(=O)NC1CCCCCCC1
Mol. weight [g/mol]:	198.31
CAS:	2163-69-1

Physical Properties

Property code	Value	Unit	Source
gf	113.24	kJ/mol	Joback Method
hf	-219.95	kJ/mol	Joback Method
hfus	21.60	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-2.22		Estimated Solubility Method
log10ws	-2.36		Aqueous Solubility Prediction Method
logp	2.370		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	595.65	K	Joback Method
tc	811.47	K	Joback Method
tf	349.13	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.71	J/mol×K	595.65	Joback Method
cpg	494.59	J/mol×K	631.62	Joback Method
cpg	514.19	J/mol×K	667.59	Joback Method
cpg	532.52	J/mol×K	703.56	Joback Method
cpg	549.62	J/mol×K	739.53	Joback Method
cpg	565.51	J/mol×K	775.50	Joback Method
cpg	580.23	J/mol×K	811.47	Joback Method

Sources

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=C2163691&Units=SI
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

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