Urea, N,N'-diphenyl-

Other names:	1,3-Diphenylcarbamide
	1,3-Diphenylurea
	AD 30
	Acardite
	Acardite I
	Carbanilide
	Diphenylcarbamide
	Diphenylurea
	Karbanilid
	N,N'-Difenylmocovina
	N,N'-Diphenylurea
	N-Phenyl-N'-phenylurea
	NSC 227401
	USAF EK-534
	Urea, 1,3-diphenyl-
	s-Diphenylurea
	sym-Diphenylurea
Inchi:	InChI=1S/C13H12N2O/c16-13(14-11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1-10H,(H2,14,1
InchiKey:	GWEHVDNNLFDJLR-UHFFFAOYSA-N
Formula:	C13H12N2O
SMILES:	O=C(Nc1ccccc1)Nc1ccccc1
Mol. weight [g/mol]:	212.25
CAS:	102-07-8

Physical Properties

Property code	Value	Unit	Source
gf	333.26	kJ/mol	Joback Method
hf	155.77	kJ/mol	Joback Method
hfs	-116.80 ± 4.40	kJ/mol	NIST Webbook
hfus	29.30	kJ/mol	Joback Method
hvap	68.70	kJ/mol	Joback Method
log10ws	-3.15		Aqueous Solubility Prediction Method
log10ws	-3.15		Estimated Solubility Method
logp	3.331		Crippen Method
mcvol	168.040	ml/mol	McGowan Method

pc	3399.94	kPa	Joback Method
tb	535.20	K	NIST Webbook
tc	950.32	K	Joback Method
tf	512.10 ± 3.00	K	NIST Webbook
tf	510.15 ± 2.00	K	NIST Webbook
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.95	J/mol×K	909.33	Joback Method
cpg	506.48	J/mol×K	950.32	Joback Method
cpg	440.45	J/mol×K	704.41	Joback Method
cpg	454.21	J/mol×K	745.39	Joback Method
cpg	466.76	J/mol×K	786.38	Joback Method
cpg	478.18	J/mol×K	827.36	Joback Method
cpg	488.54	J/mol×K	868.35	Joback Method
hfust	34.60	kJ/mol	512.00	NIST Webbook
hfust	34.62	kJ/mol	512.10	NIST Webbook
hfust	34.62	kJ/mol	512.10	NIST Webbook
hfust	34.62	kJ/mol	512.10	NIST Webbook
hsubt	152.00 ± 6.00	kJ/mol	464.50	NIST Webbook
sfust	66.50	J/mol×K	512.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102078&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
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

Legend

cpg: Ideal gas heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume