N,N-DIPHENYLUREA

Other names: Diphenyl urea
Urea, 1,1-diphenyl-
1,1-Diphenylurea
Asym-diphenylurea
Inchi: InChI=1S/C13H12N2O/c14-13(16)15(11-7-3-1-4-8-11)12-9-5-2-6-10-12/h1-10H,(H2,14,1
InchiKey: XKAFKUGMXFMRCC-UHFFFAOYSA-N
Formula: C13H12N2O
SMILES: NC(=O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 212.25

Physical Properties

Property code	Value	Unit	Source
chs	-6707.90 ± 3.30	kJ/mol	NIST Webbook
chs	-6782.70	kJ/mol	NIST Webbook
hf	6.40	kJ/mol	Cheméo Relay (1.0)
hfs	-54.40	kJ/mol	NIST Webbook
hfs	-122.70 ± 3.40	kJ/mol	NIST Webbook
hfus	27.33	kJ/mol	Joback Method
hvap	79.65	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-3.37		Cheméo Relay (1.0)
logp	2.903		Crippen Method
mcvol	168.040	ml/mol	McGowan Method
tb	593.36	K	Cheméo Relay (1.0)
tf	463.60 ± 0.00	K	NIST Webbook
tf	463.60 ± 0.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.23	J/mol×K	689.04	Joback Method
cpg	451.53	J/mol×K	731.27	Joback Method
cpg	464.50	J/mol×K	773.50	Joback Method
cpg	476.26	J/mol×K	815.73	Joback Method

cpg	486.91	J/mol×K	857.97	Joback Method
cpg	496.56	J/mol×K	900.20	Joback Method
cpg	505.31	J/mol×K	942.43	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C603543&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point