

1-Methyl-3,3-diphenylurea

Other names:	Urea, N'-methyl-N,N-diphenyl- N,N-Diphenyl-N'-methylurea 3-methyl-1,1-diphenylurea
Inchi:	InChI=1S/C14H14N2O/c1-15-14(17)16(12-8-4-2-5-9-12)13-10-6-3-7-11-13/h2-11H,1H3,(
InchiKey:	IMFYAZJNDOZIFV-UHFFFAOYSA-N
Formula:	C14H14N2O
SMILES:	CNC(=O)N(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	226.27
CAS:	13114-72-2

Physical Properties

Property code	Value	Unit	Source
chs	-7403.20 ± 7.10	kJ/mol	NIST Webbook
chs	-7465.10	kJ/mol	NIST Webbook
gf	363.07	kJ/mol	Joback Method
hf	149.19	kJ/mol	Joback Method
hfs	-106.80 ± 7.10	kJ/mol	NIST Webbook
hfus	29.82	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.164		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	689.56	K	Joback Method
tc	929.25	K	Joback Method
tf	444.40 ± 0.00	K	NIST Webbook
vc	0.662	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.59	J/mol×K	689.56	Joback Method
cpg	494.80	J/mol×K	729.51	Joback Method
cpg	508.72	J/mol×K	769.46	Joback Method

cpg	521.44	J/mol×K	809.41	Joback Method
cpg	533.05	J/mol×K	849.36	Joback Method
cpg	543.65	J/mol×K	889.30	Joback Method
cpg	553.32	J/mol×K	929.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13114722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

chs:	Standard solid enthalpy of combustion
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
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

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