Urea, N,N'-dimethyl-N,N'-diphenyl-

Other names:	1,3-dimethyl-1,3-diphenylurea CENTRALITE 2 CENTRALITE 2(dimethyldiphenyl urea) CENTRALITE II CENTRALITE II(dimethyldiphenyl urea) Carbanilide, N,N'-dimethyl- Centralit II Centralite-2 N,N'-Dimethyl-N,N'-diphenylurea N,N'-Dimethylcarbanilide NSC 59781 Zentralit II methyl centralite
Inchi:	InChI=1S/C15H16N2O/c1-16(13-9-5-3-6-10-13)15(18)17(2)14-11-7-4-8-12-14/h3-12H,1-
InchiKey:	ADCBKYIHQQCFHE-UHFFFAOYSA-N
Formula:	C15H16N2O
SMILES:	CN(C(=O)N(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	240.30
CAS:	611-92-7

Physical Properties

Property code	Value	Unit	Source
chs	-8137.50	kJ/mol	NIST Webbook
chs	-8116.10 ± 7.90	kJ/mol	NIST Webbook
chs	-8075.00	kJ/mol	NIST Webbook
gf	392.88	kJ/mol	Joback Method
hf	142.61	kJ/mol	Joback Method
hfs	-73.10 ± 7.90	kJ/mol	NIST Webbook
hfus	33.47	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hvap	64.37	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	3.379		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method

rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	674.71	K	Joback Method
tc	908.24	K	Joback Method
tf	394.60 ± 0.00	K	NIST Webbook
tf	393.15	K	DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.51	J/mol×K	674.71	Joback Method
cpg	534.18	J/mol×K	713.63	Joback Method
cpg	549.48	J/mol×K	752.55	Joback Method
cpg	563.51	J/mol×K	791.47	Joback Method
cpg	576.37	J/mol×K	830.40	Joback Method
cpg	588.16	J/mol×K	869.32	Joback Method
cpg	598.98	J/mol×K	908.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C611927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures:	https://www.doi.org/10.1016/j.jct.2010.03.025
DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers:	https://www.doi.org/10.1016/j.tca.2013.04.021
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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