N,N'-Diethyl-N,N'-diphenylurea

Other names:	1,3-Diethyl-1,3-difenylmocovina
	1,3-diethyl-1,3-diphenylurea
	1,3-diethyldiphenylurea
	Bis(N-ethyl-N-phenyl)urea
	Bis-(N-ethyl-N-fenyl)mocovina
	Carbamite
	Carbanilide, N,N'-diethyl-
	Centralite
	Centralite 1
	Centralite I
	N,N'-diethylcarbanilide
	N,N-Diethylcarbanilide
	NSC 44038
	USAF EK-1047
	Urea, 1,3-diethyl-1,3-diphenyl-
	Urea, N,N'-diethyl-N,N'-diphenyl-
	ethyl centralite
	s-Diethyldiphenylurea
	sym-Diethyldiphenylurea
Inchi:	InChI=1S/C17H20N2O/c1-3-18(15-11-7-5-8-12-15)17(20)19(4-2)16-13-9-6-10-14-16/h5-1
InchiKey:	PZIMIYVOZBTARW-UHFFFAOYSA-N
Formula:	C17H20N2O
SMILES:	CCN(C(=O)N(CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	268.35
CAS:	85-98-3

Physical Properties

Property code	Value	Unit	Source
chs	-9427.00	kJ/mol	NIST Webbook
chs	-9442.03	kJ/mol	NIST Webbook
chs	-9506.13	kJ/mol	NIST Webbook
chs	-9514.80	kJ/mol	NIST Webbook
gf	409.72	kJ/mol	Joback Method
hf	101.33	kJ/mol	Joback Method

hfus	33.54	kJ/mol	Measurement and prediction of (solid + liquid) equilibria of gun powder's and propellant's stabilizers mixtures
hvap	68.82	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	4.159		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1882.00		NIST Webbook
tb	720.47	K	Joback Method
tc	945.49	K	Joback Method
tf	345.02	K	DSC measurement and prediction of phase diagrams for binary mixtures of energetic materials' stabilizers
tf	345.70	K	Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters-based energetic materials
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.46	J/mol×K	720.47	Joback Method
cpg	641.56	J/mol×K	757.97	Joback Method
cpg	657.34	J/mol×K	795.48	Joback Method
cpg	671.90	J/mol×K	832.98	Joback Method
cpg	685.33	J/mol×K	870.49	Joback Method
cpg	697.73	J/mol×K	907.99	Joback Method
cpg	709.20	J/mol×K	945.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85983&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and modeling studies of binary organic eutectic systems to be used as stabilizers for nitrate esters-based energetic materials:	https://www.doi.org/10.1016/j.fluid.2019.06.021
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

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
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