

Urea, N-ethyl-N'-phenyl-

Other names:	Urea, 1-ethyl-3-phenyl- N-Phenyl-N'-ethylurea 1-Ethyl-3-phenylurea N-Ethyl-N'-phenylurea
Inchi:	InChI=1S/C9H12N2O/c1-2-10-9(12)11-8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H2,10,11,12)
InchiKey:	XUFXDODGXLVPNJ-UHFFFAOYSA-N
Formula:	C9H12N2O
SMILES:	CCNC(=O)Nc1ccccc1
Mol. weight [g/mol]:	164.20
CAS:	621-04-5

Physical Properties

Property code	Value	Unit	Source
gf	187.17	kJ/mol	Joback Method
hf	1.80	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Joback Method
hvap	57.52	kJ/mol	Joback Method
ie	8.25 ± 0.05	eV	NIST Webbook
log10ws	-2.26		Crippen Method
logp	1.828		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
tb	586.21	K	Joback Method
tc	804.70	K	Joback Method
tf	372.86	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.96	J/mol×K	586.21	Joback Method
cpg	337.88	J/mol×K	622.63	Joback Method
cpg	349.94	J/mol×K	659.04	Joback Method
cpg	361.17	J/mol×K	695.46	Joback Method

cpg	371.61	J/mol×K	731.87	Joback Method
cpg	381.30	J/mol×K	768.29	Joback Method
cpg	390.28	J/mol×K	804.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
ie:	Ionization energy
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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