Urea, N-methyl-N'-phenyl-

Other names:	Urea, 1-methyl-3-phenyl-
	Defenuron
	N-Methyl-N'-phenylurea
	N-Phenyl-N'-methylurea
	1-Methyl-3-phenylurea
Inchi:	InChI=1S/C8H10N2O/c1-9-8(11)10-7-5-3-2-4-6-7/h2-6H,1H3,(H2,9,10,11)
InchiKey:	SQBHGDSDVWCPHN-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CNC(=O)Nc1ccccc1
Mol. weight [g/mol]:	150.18
CAS:	1007-36-9

Physical Properties

Property code	Value	Unit	Source
gf	178.75	kJ/mol	Joback Method
hf	22.44	kJ/mol	Joback Method
hfus	22.31	kJ/mol	Joback Method
hvap	55.30	kJ/mol	Joback Method
ie	8.50 ± 0.05	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	1.438		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	563.33	K	Joback Method
tc	785.80	K	Joback Method
tf	361.59	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.91	J/mol×K	563.33	Joback Method
cpg	291.01	J/mol×K	600.41	Joback Method
cpg	302.28	J/mol×K	637.49	Joback Method

cpg	312.75	J/mol×K	674.57	Joback Method
cpg	322.47	J/mol×K	711.64	Joback Method
cpg	331.46	J/mol×K	748.72	Joback Method
cpg	339.78	J/mol×K	785.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1007369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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