Thiourea, N-methyl-N'-phenyl-

Other names:	Urea, 1-methyl-3-phenyl-2-thio-
	N-Methyl-N'-phenylthiourea
	1-Methyl-3-phenylthiocarbamide
	1-Methyl-3-phenylthiourea
	1-Phenyl-3-methylthiourea
	1-Methyl-3-phenyl-2-thiourea
Inchi:	InChI=1S/C8H10N2S/c1-9-8(11)10-7-5-3-2-4-6-7/h2-6H,1H3,(H2,9,10,11)
InchiKey:	IGEQFPWPMCIYDF-UHFFFAOYSA-N
Formula:	C8H10N2S
SMILES:	CNC(=S)Nc1ccccc1
Mol. weight [g/mol]:	166.24
CAS:	2724-69-8

Physical Properties

Property code	Value	Unit	Source
gf	424.73	kJ/mol	Joback Method
hf	281.52	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
ie	8.05 ± 0.05	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	1.603		Crippen Method
mcvol	131.830	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	579.50	K	Joback Method
tc	818.99	K	Joback Method
tf	345.93	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.01	J/mol×K	579.50	Joback Method

cpg	304.98	J/mol×K	619.42	Joback Method
cpg	315.95	J/mol×K	659.33	Joback Method
cpg	326.02	J/mol×K	699.25	Joback Method
cpg	335.28	J/mol×K	739.16	Joback Method
cpg	343.82	J/mol×K	779.08	Joback Method
cpg	351.74	J/mol×K	818.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2724698&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