Thiourea, phenyl-

Other names:	1-Phenyl-2-Thiourea
	1-Phenylthiourea
	Fenylthiomocovina
	N-Phenylthiourea
	NCI-C02017
	NSC 5779
	PTU
	Phenyl-2-thiourea
	Phenylthiocarbamide
	Phenylthiourea
	Rcra waste number P093
	Thiourea, N-phenyl-
	U 6324
	USAF EK-1569
	Urea, 1-phenyl-2-thio-
	«alpha»-Phenylthiourea
	Â«alphaÂ»-Phenylthiourea
Inchi:	InChI=1S/C7H8N2S/c8-7(10)9-6-4-2-1-3-5-6/h1-5H,(H3,8,9,10)
InchiKey:	FULZLIGZKMKICU-UHFFFAOYSA-N
Formula:	C7H8N2S
SMILES:	NC(=S)Nc1ccccc1
Mol. weight [g/mol]:	152.22
CAS:	103-85-5

Physical Properties

Property code	Value	Unit	Source
gf	393.37	kJ/mol	Joback Method
hf	282.48	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
ie	8.10	eV	NIST Webbook
log10ws	-1.77		Aqueous Solubility Prediction Method
log10ws	-1.77		Estimated Solubility Method
logp	1.342		Crippen Method
mcvol	117.740	ml/mol	McGowan Method

pc	5123.98	kPa	Joback Method
tb	578.98	K	Joback Method
tc	833.73	K	Joback Method
tf	424.65	K	Aqueous Solubility Prediction Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.93	J/mol×K	578.98	Joback Method
cpg	266.51	J/mol×K	621.44	Joback Method
cpg	276.11	J/mol×K	663.90	Joback Method
cpg	284.83	J/mol×K	706.35	Joback Method
cpg	292.79	J/mol×K	748.81	Joback Method
cpg	300.08	J/mol×K	791.27	Joback Method
cpg	306.81	J/mol×K	833.73	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103855&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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