Thiourea, N-(1-methylethyl)-N'-phenyl-

Other names:	Urea, 1-isopropyl-3-phenyl-2-thio-
	N-Phenyl-N'-isopropylthiourea
Inchi:	InChI=1S/C10H14N2S/c1-8(2)11-10(13)12-9-6-4-3-5-7-9/h3-8H,1-2H3,(H2,11,12,13)
InchiKey:	LFBMRUOVWMEFFZ-UHFFFAOYSA-N
Formula:	C10H14N2S
SMILES:	CC(C)NC(=S)Nc1ccccc1
Mol. weight [g/mol]:	194.30
CAS:	15093-36-4

Physical Properties

Property code	Value	Unit	Source
gf	439.13	kJ/mol	Joback Method
hf	234.96	kJ/mol	Joback Method
hfus	26.98	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Joback Method
ie	7.90 ± 0.05	eV	NIST Webbook
log10ws	-3.38		Crippen Method
logp	2.381		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	624.82	K	Joback Method
tc	859.68	K	Joback Method
tf	353.47	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.39	J/mol×K	624.82	Joback Method
cpg	401.19	J/mol×K	663.96	Joback Method
cpg	413.93	J/mol×K	703.11	Joback Method
cpg	425.71	J/mol×K	742.25	Joback Method
cpg	436.62	J/mol×K	781.39	Joback Method
cpg	446.76	J/mol×K	820.54	Joback Method

cpg	456.21	J/mol×K	859.68	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=C15093364&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