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

Other names: Urea, 1-tert-butyl-3-phenyl-2-thio-
Inchi: InChI=1S/C11H16N2S/c1-11(2,3)13-10(14)12-9-7-5-4-6-8-9/h4-8H,1-3H3,(H2,12,13,14)
InchiKey: JHMCTNQTJNGVRX-UHFFFAOYSA-N
Formula: C11H16N2S
SMILES: CC(C)(C)NC(S)=Nc1ccccc1
Mol. weight [g/mol]: 208.32
CAS: 14327-04-9

Physical Properties

Property code	Value	Unit	Source
hf	121.79	kJ/mol	Joback Method
hvap	57.63	kJ/mol	Joback Method
ie	7.85 ± 0.05	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	2.992		Crippen Method
mcvol	174.100	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
tb	664.12	K	Joback Method
tc	920.22	K	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=C14327049&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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