3-(4-Chlorophenyl)-1,1-dimethyl-2-thiourea

Other names: Thiourea, N'-(4-chlorophenyl)-N,N-dimethyl-
1-p-Chlorophenyl-3,3-dimethyl-2-thiourea
Inchi: InChI=1S/C9H11ClN2S/c1-12(2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
InchiKey: FWGDAHLBEXSAPT-UHFFFAOYSA-N
Formula: C9H11ClN2S
SMILES: CN(C)C(=S)Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 214.72
CAS: 2212-17-1

Physical Properties

Property code	Value	Unit	Source
gf	432.98	kJ/mol	Joback Method
hf	247.73	kJ/mol	Joback Method
hfus	29.64	kJ/mol	Joback Method
hvap	58.16	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.598		Crippen Method
mcvol	158.160	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	607.06	K	Joback Method
tc	844.06	K	Joback Method
tf	379.45	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.51	J/mol×K	607.06	Joback Method
cpg	363.73	J/mol×K	646.56	Joback Method
cpg	374.96	J/mol×K	686.06	Joback Method
cpg	385.29	J/mol×K	725.56	Joback Method
cpg	394.82	J/mol×K	765.06	Joback Method
cpg	403.64	J/mol×K	804.56	Joback Method
cpg	411.86	J/mol×K	844.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2212171&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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