2-Thiourea, 1-ethyl-1-phenyl-

Inchi: InChI=1S/C9H12N2S/c1-2-11(9(10)12)8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H2,10,12)
InchiKey: XVNPNGPNQJUMSL-UHFFFAOYSA-N
Formula: C9H12N2S
SMILES: CCN(C(N)=S)c1ccccc1
Mol. weight [g/mol]: 180.27
CAS: 3955-58-6

Physical Properties

Property code	Value	Unit	Source
gf	431.60	kJ/mol	Joback Method
hf	255.26	kJ/mol	Joback Method
hfus	25.93	kJ/mol	Joback Method
hvap	57.32	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	1.756		Crippen Method
mcvol	145.920	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	587.01	K	Joback Method
tc	828.76	K	Joback Method
tf	367.61	K	Joback Method
vc	0.514	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.97	J/mol×K	587.01	Joback Method
cpg	350.23	J/mol×K	627.30	Joback Method
cpg	362.37	J/mol×K	667.59	Joback Method
cpg	373.51	J/mol×K	707.88	Joback Method
cpg	383.74	J/mol×K	748.17	Joback Method
cpg	393.18	J/mol×K	788.47	Joback Method
cpg	401.93	J/mol×K	828.76	Joback Method

Sources

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=C3955586&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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