N,N-(Dimethyl)thiobenzamide

Other names: Benzenecarbothioamide, N,N-dimethyl-
Benzamide, N,N-dimethylthio-
Inchi: InChI=1S/C9H11NS/c1-10(2)9(11)8-6-4-3-5-7-8/h3-7H,1-2H3
InchiKey: OPXCUUJACRRYMC-UHFFFAOYSA-N
Formula: C9H11NS
SMILES: CN(C)C(=S)c1ccccc1
Mol. weight [g/mol]: 165.25
CAS: 15482-60-7

Physical Properties

Property code	Value	Unit	Source
chs	-5757.00 ± 1.40	kJ/mol	NIST Webbook
gf	365.15	kJ/mol	Joback Method
hf	136.10 ± 2.80	kJ/mol	NIST Webbook
hfs	41.30 ± 1.90	kJ/mol	NIST Webbook
hfus	20.73	kJ/mol	Joback Method
hsub	94.80 ± 2.00	kJ/mol	NIST Webbook
hvap	74.00 ± 4.00	kJ/mol	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	-2.22		Crippen Method
logp	1.924		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	514.48	K	Joback Method
tc	747.48	K	Joback Method
tf	284.35	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.60	J/mol×K	514.48	Joback Method
cpg	295.64	J/mol×K	553.31	Joback Method
cpg	308.53	J/mol×K	592.15	Joback Method

cpg	320.36	J/mol×K	630.98	Joback Method
cpg	331.24	J/mol×K	669.81	Joback Method
cpg	341.25	J/mol×K	708.65	Joback Method
cpg	350.48	J/mol×K	747.48	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=C15482607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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