Benzenamine, 4,4'-thiobis-

Other names:	Aniline, 4,4'-thiodi-
	p,p-Thiodianiline
	p,p'-Diaminodiphenyl sulfide
	Bis(4-aminophenyl) sulfide
	Di(p-aminophenyl) sulfide
	Thioaniline
	Thiodi-p-phenylenediamine
	4,4'-Diaminodiphenyl sulfide
	4,4'-Diaminophenyl sulfide
	4,4'-Thiodianiline
	Bis(p-aminophenyl)sulfide
	NCI-C01707
	Sulfide, bis(p-aminophenyl)
	4,4'-Thioaniline
	4,4'-Thiobisbenzenamine
	4,4'-Thiobis(aniline)
	Bis(p-aminophenyl)sulphide
	Bis(4-aminophenyl)sulphide
	p,p'-Diaminodiphenyl sulphide
	4,4-Diaminodiphenyl sulphide
	4,4'-Diaminodiphenylsulphide
	Di(p-aminophenyl)sulphide
	NSC 6191
Inchi:	InChI=1S/C12H12N2S/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H,13-14H2
InchiKey:	ICNFHJVPAJKPHW-UHFFFAOYSA-N
Formula:	C12H12N2S
SMILES:	Nc1ccc(Sc2ccc(N)cc2)cc1
Mol. weight [g/mol]:	216.30
CAS:	139-65-1

Physical Properties

Property code	Value	Unit	Source
gf	421.74	kJ/mol	Joback Method
hf	268.56	kJ/mol	Joback Method
hfus	28.66	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method

ie	6.75	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	3.002		Crippen Method
mcvol	168.730	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	751.12	K	Joback Method
tc	1032.77	K	Joback Method
tf	503.80	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.53	J/mol×K	751.12	Joback Method
cpg	451.61	J/mol×K	798.06	Joback Method
cpg	463.37	J/mol×K	845.00	Joback Method
cpg	473.89	J/mol×K	891.95	Joback Method
cpg	483.25	J/mol×K	938.89	Joback Method
cpg	491.52	J/mol×K	985.83	Joback Method
cpg	498.79	J/mol×K	1032.77	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C139651&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

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