Benzenamine, 3-(methylthio)-

Other names:	3-(Methylthio)aniline
	3-Methylthiobenzenamine
	3-Methylmercaptoaniline
	m-(Methylthio)aniline
	m-Aminophenyl methyl sulfide
	m-Aminothioanisole
	Aniline, m-(methylthio)-
	3-Aminothioanisole
	Aniline, 3-methylthio-
	3-CH3SC6H4NH2
	3-(Methylsulfanyl)phenylamine
	NSC 66274
Inchi:	InChI=1S/C7H9NS/c1-9-7-4-2-3-6(8)5-7/h2-5H,8H2,1H3
InchiKey:	KCHLDNLIJVSRPK-UHFFFAOYSA-N
Formula:	C7H9NS
SMILES:	CSc1cccc(N)c1
Mol. weight [g/mol]:	139.22
CAS:	1783-81-9

Physical Properties

Property code	Value	Unit	Source
affp	902.10	kJ/mol	NIST Webbook
basg	870.30	kJ/mol	NIST Webbook
gf	210.41	kJ/mol	Joback Method
hf	112.91	kJ/mol	Joback Method
hfus	16.86	kJ/mol	Joback Method
hvap	51.57	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.991		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	4444.44	kPa	Joback Method
tb	532.53	K	Joback Method
tc	783.92	K	Joback Method
tf	325.25	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.94	J/mol×K	532.53	Joback Method
cpg	243.64	J/mol×K	574.43	Joback Method
cpg	254.54	J/mol×K	616.33	Joback Method
cpg	264.66	J/mol×K	658.23	Joback Method
cpg	274.04	J/mol×K	700.13	Joback Method
cpg	282.69	J/mol×K	742.02	Joback Method
cpg	290.64	J/mol×K	783.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	437.20	K	2.10	NIST Webbook
tbrp	437.00 ± 1.00	K	2.10	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1783819&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume