Benzenamine, 2-methyl-N-sulfinyl-

Other names:	o-Toluidine, N-sulfinyl-
	o-Tolylsulfinylamine
	N-Sulfinyl-o-toluidine
	Thionyl-o-toluidine
	2-Methyl-N-sulfinylaniline
	2-Methylsulfinylaniline
	2-Methyl-N-sulfinylbenzenamine
Inchi:	InChI=1S/C7H7NOS/c1-6-4-2-3-5-7(6)8-10-9/h2-5H,1H3
InchiKey:	XYPGFEPVLMKJKM-UHFFFAOYSA-N
Formula:	C7H7NOS
SMILES:	Cc1ccccc1N=S=O
Mol. weight [g/mol]:	153.20
CAS:	15182-74-8

Physical Properties

Property code	Value	Unit	Source
hf	-89.07	kJ/mol	Joback Method
hvap	50.03	kJ/mol	Joback Method
ie	8.75	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	2.023		Crippen Method
mcvol	113.630	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	523.40	K	Joback Method
tc	757.93	K	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=C15182748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation 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