3-Thiophenamine, tetrahydro-N-methyl-N-nitroso-, 1,1-dioxide

Other names: N-Methyl-N-nitroso-3-tetrahydrothiophenamine 1,1-dioxide
N-Nitrosomethylaminosulfolane
Phenamine, tetrahydro-N-methyl-N-nitroso-3-thio-, 1,1-dioxide
Tetrahydro-N-methyl-N-nitroso-3-thiophenamine 1,1-dioxide
3-(N-Nitrosomethylamino)sulfolan
3-Thiophenine, tetrahydro-N-methyl-N-nitroso-, 1,1-dioxide

Inchi: InChI=1S/C5H10N2O3S/c1-7(6-8)5-2-3-11(9,10)4-5/h5H,2-4H2,1H3

InchiKey: PRZXZYVFNZCXQH-UHFFFAOYSA-N

Formula: C5H10N2O3S

SMILES: CN(N=O)C1CCS(=O)(=O)C1

Mol. weight [g/mol]: 178.21

CAS: 13256-21-8

Physical Properties

Property code	Value	Unit	Source
hf	-636.67	kJ/mol	Joback Method
hvap	55.75	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	-0.213		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	431.75	K	Joback Method
tc	615.13	K	Joback Method

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=C13256218&Units=SI

Legend

hf:	Enthalpy of formation 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