Ethenamine, N-methyl-1-(methylthio)-2-nitro-

Other names: N-Methyl-1-methylthio-2-nitro-1-etheneamine
N-methyl-1-(methylthio)-2-nitrovinylamine
Inchi: InChI=1S/C4H8N2O2S/c1-5-4(9-2)3-6(7)8/h3,5H,1-2H3/b4-3+
InchiKey: YQFHPXZGXNYYLD-ONEGZZNKSA-N
Formula: C4H8N2O2S
SMILES: CNC(=C[N+](=O)[O-])SC
Mol. weight [g/mol]: 148.18
CAS: 61832-41-5

Physical Properties

Property code	Value	Unit	Source
gf	212.53	kJ/mol	Joback Method
hf	66.12	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	54.38	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	0.644		Crippen Method
mcvol	106.670	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	565.75	K	Joback Method
tc	810.46	K	Joback Method
tf	346.47	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.44	J/mol×K	565.75	Joback Method
cpg	242.02	J/mol×K	606.54	Joback Method
cpg	250.92	J/mol×K	647.32	Joback Method
cpg	259.16	J/mol×K	688.11	Joback Method
cpg	266.79	J/mol×K	728.89	Joback Method
cpg	273.84	J/mol×K	769.68	Joback Method
cpg	280.35	J/mol×K	810.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61832415&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
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