N-METHYL-1-METHYLTHIO-2-NITRO-1-ETHENEAI

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: CN/C(=C\[N+](=O)[O-])SC
Mol. weight [g/mol]: 148.19

Physical Properties

Property code	Value	Unit	Source
hfus	25.60	kJ/mol	Joback Method
logp	0.644		Crippen Method
mcvol	106.670	ml/mol	McGowan 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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61832415&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume