Ethanethioamide, N,N-dimethyl-

Other names:	Acetamide, N,N-dimethylthio-
	Dimethylthioacetamide
	N,N-Dimethylthioacetamide
	Dimethylthioacetamid
	N,N-dimethylethanethioamide
Inchi:	InChI=1S/C4H9NS/c1-4(6)5(2)3/h1-3H3
InchiKey:	LKNQXZAHNDFIQY-UHFFFAOYSA-N
Formula:	C4H9NS
SMILES:	CC(=S)N(C)C
Mol. weight [g/mol]:	103.19
CAS:	631-67-4

Physical Properties

Property code	Value	Unit	Source
affp	925.30	kJ/mol	NIST Webbook
basg	894.40	kJ/mol	NIST Webbook
gf	210.64	kJ/mol	Joback Method
hf	88.14	kJ/mol	Joback Method
hfus	13.74	kJ/mol	Joback Method
hvap	33.27	kJ/mol	Joback Method
ie	7.86	eV	NIST Webbook
log10ws	-0.92		Crippen Method
logp	0.895		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	4374.18	kPa	Joback Method
tb	373.40	K	Joback Method
tc	568.30	K	Joback Method
tf	201.58	K	Joback Method
vc	0.314	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.86	J/mol×K	373.40	Joback Method

cpg	157.40	J/mol×K	405.88	Joback Method
cpg	166.32	J/mol×K	438.37	Joback Method
cpg	174.64	J/mol×K	470.85	Joback Method
cpg	182.41	J/mol×K	503.33	Joback Method
cpg	189.65	J/mol×K	535.82	Joback Method
cpg	196.42	J/mol×K	568.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.00 ± 1.00	K	2.90	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=C631674&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
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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume