Methanethioamide, N,N-dimethyl-

Other names:	Formamide, N,N-dimethylthio-
	Dimethylthioformamide
	N,N-Dimethylthioformamide
	HCSN(CH3)2
	N,N-Dimethylmethanethioamide
	N,N-dimethylthioforamide
Inchi:	InChI=1S/C3H7NS/c1-4(2)3-5/h3H,1-2H3
InchiKey:	SKECXRFZFFAANN-UHFFFAOYSA-N
Formula:	C3H7NS
SMILES:	CN(C)C=S
Mol. weight [g/mol]:	89.16
CAS:	758-16-7

Physical Properties

Property code	Value	Unit	Source
affp	906.40	kJ/mol	NIST Webbook
basg	875.50	kJ/mol	NIST Webbook
gf	210.77	kJ/mol	Joback Method
hf	118.57	kJ/mol	Joback Method
hfus	12.46	kJ/mol	Joback Method
hvap	30.96	kJ/mol	Joback Method
ie	8.16	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-0.50		Crippen Method
logp	0.505		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
ripol	1829.00		NIST Webbook
ripol	1829.00		NIST Webbook
tb	350.64	K	Joback Method
tc	542.31	K	Joback Method
tf	204.27	K	Joback Method
vc	0.257	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.47	J/mol×K	350.64	Joback Method
cpg	122.44	J/mol×K	382.58	Joback Method
cpg	129.85	J/mol×K	414.53	Joback Method
cpg	136.75	J/mol×K	446.47	Joback Method
cpg	143.16	J/mol×K	478.42	Joback Method
cpg	149.12	J/mol×K	510.36	Joback Method
cpg	154.66	J/mol×K	542.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.00 ± 1.00	K	3.60	NIST Webbook

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=C758167&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume