N,N-Dimethylthioformamide

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

Physical Properties

Property code	Value	Unit	Source
affp	906.40	kJ/mol	NIST Webbook
basg	875.50	kJ/mol	NIST Webbook
hfus	12.46	kJ/mol	Joback Method
ie	8.16	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
logp	0.505		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
ripol	1829.00		NIST Webbook
ripol	1829.00		NIST Webbook

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C758167&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

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices
tbrp: Boiling point at reduced pressure