CH3OC(S)N(CH3)2

Inchi: InChI=1S/C4H9NOS/c1-5(2)4(7)6-3/h1-3H3
InchiKey: QPKDBLGFWZSDSB-UHFFFAOYSA-N
Formula: C4H9NOS
SMILES: COC(=S)N(C)C
Mol. weight [g/mol]: 119.19
CAS: 16703-45-0

Physical Properties

Property code	Value	Unit	Source
affp	900.00	kJ/mol	NIST Webbook
basg	869.00	kJ/mol	NIST Webbook
gf	105.64	kJ/mol	Joback Method
hf	-44.08	kJ/mol	Joback Method
hfus	14.93	kJ/mol	Joback Method
hvap	35.68	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.479		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	395.82	K	Joback Method
tc	590.61	K	Joback Method
tf	223.81	K	Joback Method
vc	0.332	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.99	J/mol×K	395.82	Joback Method
cpg	178.10	J/mol×K	428.28	Joback Method
cpg	186.70	J/mol×K	460.75	Joback Method
cpg	194.80	J/mol×K	493.21	Joback Method
cpg	202.43	J/mol×K	525.68	Joback Method
cpg	209.63	J/mol×K	558.14	Joback Method
cpg	216.41	J/mol×K	590.61	Joback Method

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=C16703450&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
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