Sulfurous acid, dimethyl ester

Other names:	(CH3O)2SO
	Dimethoxy sulfoxide
	Dimethyl ester of sulfurous acid
	Dimethyl sulfite
	Dimethyl sulphite
	Methyl sulfite
	Sulphurous acid dimethyl ester
Inchi:	InChI=1S/C2H6O3S/c1-4-6(3)5-2/h1-2H3
InchiKey:	BDUPRNVPXOHWIL-UHFFFAOYSA-N
Formula:	C2H6O3S
SMILES:	COS(=O)OC
Mol. weight [g/mol]:	110.13
CAS:	616-42-2

Physical Properties

Property code	Value	Unit	Source
chl	-1723.20 ± 0.96	kJ/mol	NIST Webbook
gf	-461.75	kJ/mol	Joback Method
hf	-483.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-523.30 ± 1.00	kJ/mol	NIST Webbook
hfus	11.07	kJ/mol	Joback Method
hvap	40.00 ± 2.00	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	10.25	eV	NIST Webbook
ie	10.25	eV	NIST Webbook
log10ws	0.55		Crippen Method
logp	-0.142		Crippen Method
mcvol	73.000	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	348.28	K	Joback Method
tc	526.76	K	Joback Method
tf	193.24	K	Joback Method
vc	0.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.87	J/mol×K	348.28	Joback Method
cpg	128.72	J/mol×K	378.03	Joback Method
cpg	133.62	J/mol×K	407.77	Joback Method
cpg	138.54	J/mol×K	437.52	Joback Method
cpg	143.47	J/mol×K	467.27	Joback Method
cpg	148.39	J/mol×K	497.01	Joback Method
cpg	153.26	J/mol×K	526.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27360e+01
Coeff. B	-2.81590e+03
Coeff. C	-5.21140e+01
Temperature range (K), min.	278.32
Temperature range (K), max.	431.59

Sources

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=C616422&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume