Sulfuric acid, dimethyl ester

Other names:	DIMETHYL MONOSULFATE
	DMS
	DMS (Methyl sulfate)
	Dimethoxysulfone
	Dimethyl sulfate
	Dimethyl sulphate
	Dimethylester kyseliny sirove
	Dimethylsulfaat
	Dimethylsulfat
	Dimetilsolfato
	Dwumetylowy siarczan
	Methyl Sulfate
	Methyl sulfate, Me2SO4
	Methyle (sulfate de)
	NSC 56194
	Rcra waste number U103
	Sulfate de dimethyle
	Sulfate dimethylique
	Sulphuric acid dimethyl ester
	UN 1595
Inchi:	InChI=1S/C2H6O4S/c1-5-7(3,4)6-2/h1-2H3
InchiKey:	VAYGXNSJCAHWJZ-UHFFFAOYSA-N
Formula:	C2H6O4S
SMILES:	COS(=O)(=O)OC
Mol. weight [g/mol]:	126.13
CAS:	77-78-1

Physical Properties

Property code	Value	Unit	Source
gf	-712.58	kJ/mol	Joback Method
hf	-687.00 ± 1.90	kJ/mol	NIST Webbook
hfl	-735.25 ± 0.92	kJ/mol	NIST Webbook
hfus	14.69	kJ/mol	Joback Method
hvap	49.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	0.35		Crippen Method
logp	-0.476		Crippen Method
mcvol	78.870	ml/mol	McGowan Method

pc	6018.58	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	853.00		NIST Webbook
tb	470.00 ± 6.00	K	NIST Webbook
tb	461.70 ± 0.60	K	NIST Webbook
tb	461.95 ± 0.30	K	NIST Webbook
tc	502.46	K	Joback Method
tf	241.40 ± 0.20	K	NIST Webbook
tf	241.15 ± 0.50	K	NIST Webbook
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.38	J/mol×K	337.78	Joback Method
cpg	141.43	J/mol×K	365.23	Joback Method
cpg	146.52	J/mol×K	392.67	Joback Method
cpg	151.63	J/mol×K	420.12	Joback Method
cpg	156.75	J/mol×K	447.57	Joback Method
cpg	161.84	J/mol×K	475.01	Joback Method
cpg	166.90	J/mol×K	502.46	Joback Method
hvapt	46.70	kJ/mol	405.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30883e+01
Coeff. B	-3.30869e+03
Coeff. C	-7.93640e+01
Temperature range (K), min.	337.84
Temperature range (K), max.	504.82

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77781&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1861.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume