Dimethyl sulfone

Other names:	DMSO2
	Dimethyl sulphone
	MSM
	Methane, 1,1'-sulfonylbis-
	Methane, sulfonylbis-
	Methyl sulfone
	Methylsulfonylmethane
	NSC 63345
	Sulfone, dimethyl-
	Sulfonylbismethane
	Sulphonylbismethane
Inchi:	InChI=1S/C2H6O2S/c1-5(2,3)4/h1-2H3
InchiKey:	HHVIBTZHLRERCL-UHFFFAOYSA-N
Formula:	C2H6O2S
SMILES:	CS(C)(=O)=O
Mol. weight [g/mol]:	94.13
CAS:	67-71-0

Physical Properties

Property code	Value	Unit	Source
chs	-1796.70 ± 0.50	kJ/mol	NIST Webbook
gf	-502.58	kJ/mol	Joback Method
hf	-373.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-446.40	kJ/mol	NIST Webbook
hfs	-449.82 ± 0.59	kJ/mol	NIST Webbook
hfus	12.31	kJ/mol	Joback Method
hsub	77.00 ± 3.00	kJ/mol	NIST Webbook
hvap	38.68	kJ/mol	Joback Method
ie	10.65	eV	NIST Webbook
ie	10.97	eV	NIST Webbook
ie	10.65	eV	NIST Webbook
ie	10.80	eV	NIST Webbook
log10ws	0.51		Crippen Method
logp	-0.339		Crippen Method
mcvol	67.130	ml/mol	McGowan Method
pc	6349.11	kPa	Joback Method
rinpol	918.00		NIST Webbook

rinpol	919.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	921.60		NIST Webbook
rinpol	914.90		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	924.00		NIST Webbook
ripol	1912.00		NIST Webbook
ripol	1900.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1887.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1911.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1913.00		NIST Webbook
ripol	1906.00		NIST Webbook
ripol	1912.00		NIST Webbook
ripol	1881.40		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1908.00		NIST Webbook
ss	145.48	J/mol×K	NIST Webbook
tb	511.00 ± 3.00	K	NIST Webbook
tc	453.77	K	Joback Method
tf	150.86	K	Joback Method
tt	382.01 ± 0.04	K	NIST Webbook
tt	382.00 ± 0.06	K	NIST Webbook
vc	0.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.97	J/mol×K	400.16	Joback Method
cpg	123.94	J/mol×K	426.96	Joback Method
cpg	98.00	J/mol×K	292.94	Joback Method
cpg	103.39	J/mol×K	319.74	Joback Method
cpg	108.69	J/mol×K	346.55	Joback Method
cpg	113.88	J/mol×K	373.35	Joback Method
cpg	128.79	J/mol×K	453.77	Joback Method
cps	125.35	J/mol×K	298.15	NIST Webbook
hfust	18.30	kJ/mol	382.01	NIST Webbook
hfust	18.28	kJ/mol	382.00	NIST Webbook
hvapt	56.00	kJ/mol	455.00	NIST Webbook
sfust	47.91	J/mol×K	382.01	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48648e+01
Coeff. B	-4.38294e+03
Coeff. C	-8.32500e+01
Temperature range (K), min.	382.05
Temperature range (K), max.	542.24

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67710&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume