Dimethylsulfoxide-D6

Other names:	(methyl sulfoxide)-d6
	Deutero-,dimethylsulfoxide
	Methane-D3-, sulfinylbis-
	di[(2H3)methyl] sulphoxide
	dimethyl-d6 sulfoxide
	hexadeuteriodimethyl sulfoxide
	sulfinylbismethane-d3
Inchi:	InChI=1S/C2H6OS/c1-4(2)3/h1-2H3/i1D3,2D3
InchiKey:	IAZDPXIOMUYVGZ-WFGJKAKNSA-N
Formula:	C2D6OS
SMILES:	CS(C)=O
Mol. weight [g/mol]:	84.17
CAS:	2206-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-251.75	kJ/mol	Joback Method
hf	-290.35	kJ/mol	Joback Method
hfus	8.69	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	0.70		Crippen Method
logp	-0.005		Crippen Method
mcvol	61.260	ml/mol	McGowan Method
pc	5704.58	kPa	Joback Method
tb	303.44	K	Joback Method
tc	478.96	K	Joback Method
tf	293.40	K	Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment
vc	0.237	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.68	J/mol×K	303.44	Joback Method
cpg	91.87	J/mol×K	332.69	Joback Method
cpg	96.95	J/mol×K	361.95	Joback Method
cpg	101.92	J/mol×K	391.20	Joback Method
cpg	106.76	J/mol×K	420.45	Joback Method
cpg	111.48	J/mol×K	449.71	Joback Method
cpg	116.06	J/mol×K	478.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2206271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Efficient determination of crystallisation and melting points at low cooling and heating rates with novel computer controlled equipment:	https://www.doi.org/10.1016/j.jct.2008.05.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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

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