

Diethyl sulfate

Other names:	DES Diaethylsulfat Diethyl sulphate Diethylester kyseliny sirove Ethyl sulfate NSC 56380 Sulfuric acid, diethyl ester Sulphuric acid diethyl ester UN 1594
Inchi:	InChI=1S/C4H10O4S/c1-3-7-9(5,6)8-4-2/h3-4H2,1-2H3
InchiKey:	DENRZWYUOJLTMF-UHFFFAOYSA-N
Formula:	C4H10O4S
SMILES:	CCOS(=O)(=O)OCC
Mol. weight [g/mol]:	154.19
CAS:	64-67-5

Physical Properties

Property code	Value	Unit	Source
chl	-2792.30 ± 0.96	kJ/mol	NIST Webbook
gf	-695.74	kJ/mol	Joback Method
hf	-756.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-812.90 ± 1.00	kJ/mol	NIST Webbook
hfus	19.87	kJ/mol	Joback Method
hvap	57.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-0.49		Crippen Method
logp	0.304		Crippen Method
mcvol	107.050	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	383.54	K	Joback Method
tc	548.25	K	Joback Method
tf	248.75	K	NIST Webbook
tf	247.15 ± 0.50	K	NIST Webbook
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.22	J/mol×K	383.54	Joback Method
cpg	209.48	J/mol×K	410.99	Joback Method
cpg	217.63	J/mol×K	438.44	Joback Method
cpg	225.65	J/mol×K	465.90	Joback Method
cpg	233.52	J/mol×K	493.35	Joback Method
cpg	241.23	J/mol×K	520.80	Joback Method
cpg	248.77	J/mol×K	548.25	Joback Method
hvapt	50.10	kJ/mol	448.50	NIST Webbook
hvapt	54.90	kJ/mol	401.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64675&Units=SI
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/mol1872.mol

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
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

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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