Sulfurous acid, diethyl ester

Other names:	(C2H5O)2SO
	DIETHYL SULPHITE
	Diethyl ester of sulfurous acid
	Diethyl sulfite
	Ethyl sulfite
	Ethyl sulfite, (Et2SO3)
	NSC 8838
	SULPHUROUS ACID DIETHYL ESTER
Inchi:	InChI=1S/C4H10O3S/c1-3-6-8(5)7-4-2/h3-4H2,1-2H3
InchiKey:	NVJBFARDFTXOTO-UHFFFAOYSA-N
Formula:	C4H10O3S
SMILES:	CCOS(=O)OCC
Mol. weight [g/mol]:	138.19
CAS:	623-81-4

Physical Properties

Property code	Value	Unit	Source
chl	-3004.80 ± 2.70	kJ/mol	NIST Webbook
gf	-444.91	kJ/mol	Joback Method
hf	-552.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-600.45 ± 0.88	kJ/mol	NIST Webbook
hfus	16.25	kJ/mol	Joback Method
hvap	49.00 ± 2.00	kJ/mol	NIST Webbook
hvap	44.50	kJ/mol	NIST Webbook
ie	9.68	eV	NIST Webbook
log10ws	-0.29		Crippen Method
logp	0.638		Crippen Method
mcvol	101.180	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	429.00 ± 5.00	K	NIST Webbook
tb	430.00 ± 1.00	K	NIST Webbook
tb	431.00 ± 2.00	K	NIST Webbook
tb	431.00 ± 1.00	K	NIST Webbook
tb	430.85 ± 0.60	K	NIST Webbook
tc	571.43	K	Joback Method
tf	215.78	K	Joback Method
vc	0.386	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.96	J/mol×K	394.04	Joback Method
cpg	197.19	J/mol×K	423.60	Joback Method
cpg	205.29	J/mol×K	453.17	Joback Method
cpg	213.26	J/mol×K	482.73	Joback Method
cpg	221.06	J/mol×K	512.30	Joback Method
cpg	228.69	J/mol×K	541.86	Joback Method
cpg	236.13	J/mol×K	571.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623814&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/mol1871.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
ie: Ionization energy
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