Endosulfan sulfate

Other names:	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3,3-dioxide 5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfate Thiodan sulfate Endosulfan sulphate 6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano-2,4,3-benzodioxathiepin-3,3-dioxide
Inchi:	InChI=1S/C9H6Cl6O4S/c10-5-6(11)8(13)4-2-19-20(16,17)18-1-3(4)7(5,12)9(8,14)15/h3-4
InchiKey:	AAPVQEMYVNZIOO-UHFFFAOYSA-N
Formula:	C9H6Cl6O4S
SMILES:	O=S1(=O)OCC2C(CO1)C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	422.93
CAS:	1031-07-8

Physical Properties

Property code	Value	Unit	Source
gf	-555.96	kJ/mol	Joback Method
hf	-797.69	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.356		Crippen Method
mcvol	214.060	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	2362.00		NIST Webbook
tb	744.16	K	Joback Method
tc	1010.72	K	Joback Method
tf	420.86 ± 0.20	K	NIST Webbook
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.69	J/mol×K	966.30	Joback Method
cpg	494.87	J/mol×K	744.16	Joback Method
cpg	506.69	J/mol×K	788.59	Joback Method

cpg	519.29	J/mol×K	833.01	Joback Method
cpg	533.28	J/mol×K	877.44	Joback Method
cpg	549.21	J/mol×K	921.87	Joback Method
cpg	589.29	J/mol×K	1010.72	Joback Method
hfust	21.66	kJ/mol	419.70	NIST Webbook
hvapt	85.60	kJ/mol	398.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1031078&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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