«alpha»-Endosulfan

Other names:	Endosulfan I
	6,9-Methano-2,4,3-benzodioxathiepin, 6,7,8,9,10,10-hexachloro-1,5,5a,6,9,9a-hexahydro-, 3-oxide, (3«alpha»,5a«beta»,6«alpha»,9«alpha»,9a«beta»)-
	5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, endo-
	«alpha»-Thiodan
	Endosulfan, «alpha»-
	Endosulfan 1
	Endosulfan A
	«alpha»-Benzoepin
	«beta»-Thionex
Inchi:	InChI=1S/C9H6Cl6O3S/c10-5-6(11)8(13)4-2-18-19(16)17-1-3(4)7(5,12)9(8,14)15/h3-4H,
InchiKey:	RDYMFSUJUZBWLH-AMHWMVONSA-N
Formula:	C9H6Cl6O3S
SMILES:	O=S1OCC2C(CO1)C1(Cl)C(Cl)=C(Cl)C2(Cl)C1(Cl)Cl
Mol. weight [g/mol]:	406.93
CAS:	959-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-305.13	kJ/mol	Joback Method
hf	-550.08	kJ/mol	Joback Method
hfus	39.28	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.690		Crippen Method
mcvol	208.190	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2086.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2150.00		NIST Webbook
ripol	2880.00		NIST Webbook

ripol	2880.00		NIST Webbook
tb	754.66	K	Joback Method
tc	1036.70	K	Joback Method
tf	381.27 ± 0.20	K	NIST Webbook
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.43	J/mol×K	754.66	Joback Method
cpg	488.77	J/mol×K	801.67	Joback Method
cpg	502.31	J/mol×K	848.67	Joback Method
cpg	517.78	J/mol×K	895.68	Joback Method
cpg	535.85	J/mol×K	942.69	Joback Method
cpg	557.24	J/mol×K	989.70	Joback Method
cpg	582.64	J/mol×K	1036.70	Joback Method
hfust	10.00	kJ/mol	380.00	NIST Webbook
hvapt	80.40	kJ/mol	398.00	NIST Webbook

Sources

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=C959988&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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