Endosulfan ether

Other names:	4,7-Methanoisobenzofuran, 4,5,6,7,8,8-hexachloro-1,3,3a,4,7,7a-hexahydro- NSC 37660
Inchi:	InChI=1S/C9H6Cl6O/c10-5-6(11)8(13)4-2-16-1-3(4)7(5,12)9(8,14)15/h3-4H,1-2H2
InchiKey:	CKPWHXBGVRURFU-UHFFFAOYSA-N
Formula:	C9H6Cl6O
SMILES:	ClC1=C(Cl)C2(Cl)C3COCC3C1(Cl)C2(Cl)Cl
Mol. weight [g/mol]:	342.86
CAS:	3369-52-6

Physical Properties

Property code	Value	Unit	Source
gf	16.16	kJ/mol	Joback Method
hf	-203.41	kJ/mol	Joback Method
hfus	28.22	kJ/mol	Joback Method
hvap	63.90	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.095		Crippen Method
mcvol	180.100	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	681.84	K	Joback Method
tc	957.96	K	Joback Method
tf	536.60	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.06	J/mol×K	681.84	Joback Method
cpg	401.89	J/mol×K	727.86	Joback Method
cpg	412.12	J/mol×K	773.88	Joback Method
cpg	423.46	J/mol×K	819.90	Joback Method
cpg	436.59	J/mol×K	865.92	Joback Method
cpg	452.24	J/mol×K	911.94	Joback Method
cpg	471.09	J/mol×K	957.96	Joback Method

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=C3369526&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
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