Hexachlorophene dimethyl ether

Inchi: InChI=1S/C15H11Cl5O2/c1-21-12-4-3-9(16)13(19)7(12)5-8-14(20)10(17)6-11(18)15(8)22
InchiKey: ZZFFLZBDRDHFBT-UHFFFAOYSA-N
Formula: C15H11Cl5O2
SMILES: COc1ccc(Cl)c(Cl)c1Cc1c(Cl)c(Cl)cc(Cl)c1OC
Mol. weight [g/mol]: 400.51

Physical Properties

Property code	Value	Unit	Source
gf	-36.82	kJ/mol	Joback Method
hf	-303.30	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	84.91	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.562		Crippen Method
mcvol	247.630	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2666.00		NIST Webbook
tb	862.81	K	Joback Method
tc	1108.45	K	Joback Method
tf	593.35	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.83	J/mol×K	862.81	Joback Method
cpg	623.17	J/mol×K	1067.51	Joback Method
cpg	617.49	J/mol×K	1026.57	Joback Method
cpg	610.71	J/mol×K	985.63	Joback Method
cpg	602.83	J/mol×K	944.69	Joback Method
cpg	593.87	J/mol×K	903.75	Joback Method
cpg	627.74	J/mol×K	1108.45	Joback Method
dvisc	0.0000643	Pa×s	862.81	Joback Method
dvisc	0.0000755	Pa×s	817.90	Joback Method

dvisc	0.0000904	Pa×s	772.99	Joback Method
dvisc	0.0001107	Pa×s	728.08	Joback Method
dvisc	0.0001391	Pa×s	683.17	Joback Method
dvisc	0.0001805	Pa×s	638.26	Joback Method
dvisc	0.0002437	Pa×s	593.35	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R543152&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume