Bis(2,3,3,3-tetrachloropropyl) ether

Other names:	Ether, bis(2,3,3,3-tetrachloropropyl)
	Monsanto 16226
	Octachloro-di-n-propyl ether
	Octachlorodipropyl ether
	Propane, 1,1'-oxybis[2,3,3,3-tetrachloro-
	S 421
	2,3,3,3,2',3',3',3'-Octachlorodipropyl ether
	ENT 25,456
	Monsanto CP-16226
Inchi:	InChI=1S/C6H6Cl8O/c7-3(5(9,10)11)1-15-2-4(8)6(12,13)14/h3-4H,1-2H2
InchiKey:	LNJXZKBHJZAIKQ-UHFFFAOYSA-N
Formula:	C6H6Cl8O
SMILES:	ClC(COCC(Cl)C(Cl)(Cl)Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	377.74
CAS:	127-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-200.00	kJ/mol	Joback Method
hf	-453.37	kJ/mol	Joback Method
hfus	24.19	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.958		Crippen Method
mcvol	199.190	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	651.20	K	Joback Method
tc	894.28	K	Joback Method
tf	393.81	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.14	J/mol×K	651.20	Joback Method
cpg	382.42	J/mol×K	691.71	Joback Method
cpg	388.89	J/mol×K	732.23	Joback Method
cpg	394.64	J/mol×K	772.74	Joback Method
cpg	399.75	J/mol×K	813.26	Joback Method
cpg	404.31	J/mol×K	853.77	Joback Method
cpg	408.40	J/mol×K	894.28	Joback Method
dvisc	0.0021357	Pa×s	393.81	Joback Method
dvisc	0.0010297	Pa×s	436.71	Joback Method
dvisc	0.0005657	Pa×s	479.61	Joback Method
dvisc	0.0003429	Pa×s	522.50	Joback Method
dvisc	0.0002242	Pa×s	565.40	Joback Method
dvisc	0.0001557	Pa×s	608.30	Joback Method
dvisc	0.0001134	Pa×s	651.20	Joback Method

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=C127902&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
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