Chlorthal

Other names:	1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-
	Terephthalic acid, tetrachloro-
	Tetrachloroterephthalic acid
	2,3,5,6-Tetrachloroterephthalic acid
	Dacthal diacid
	TCTP (terephthalic acid, tetrachloro)
Inchi:	InChI=1S/C8H2Cl4O4/c9-3-1(7(13)14)4(10)6(12)2(5(3)11)8(15)16/h(H,13,14)(H,15,16)
InchiKey:	KZCBXHSWMMIEQU-UHFFFAOYSA-N
Formula:	C8H2Cl4O4
SMILES:	O=C(O)c1c(Cl)c(Cl)c(C(=O)O)c(Cl)c1Cl
Mol. weight [g/mol]:	303.91
CAS:	2136-79-0

Physical Properties

Property code	Value	Unit	Source
gf	-498.46	kJ/mol	Joback Method
hf	-621.85	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	103.38	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.697		Crippen Method
mcvol	163.660	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
ripol	2820.00		NIST Webbook
tb	875.84	K	Joback Method
tc	1095.11	K	Joback Method
tf	610.12	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.90	J/mol×K	875.84	Joback Method
cpg	339.59	J/mol×K	912.38	Joback Method

cpg	342.87	J/mol×K	948.93	Joback Method
cpg	345.75	J/mol×K	985.47	Joback Method
cpg	348.25	J/mol×K	1022.02	Joback Method
cpg	350.36	J/mol×K	1058.56	Joback Method
cpg	352.10	J/mol×K	1095.11	Joback Method
dvisc	0.0001075	Pa×s	610.12	Joback Method
dvisc	0.0000587	Pa×s	654.41	Joback Method
dvisc	0.0000346	Pa×s	698.69	Joback Method
dvisc	0.0000217	Pa×s	742.98	Joback Method
dvisc	0.0000144	Pa×s	787.27	Joback Method
dvisc	0.0000099	Pa×s	831.55	Joback Method
dvisc	0.0000071	Pa×s	875.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2136790&Units=SI
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

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