

Propane-1,2-diyl bis(3-chlorobenzoate)

Inchi:	InChI=1S/C17H14Cl2O4/c1-11(23-17(21)13-5-3-7-15(19)9-13)10-22-16(20)12-4-2-6-14(
InchiKey:	MKQOXSIRSIFZPS-UHFFFAOYSA-N
Formula:	C17H14Cl2O4
SMILES:	CC(COC(=O)c1cccc(Cl)c1)OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	353.20

Physical Properties

Property code	Value	Unit	Source
gf	-196.32	kJ/mol	Joback Method
hf	-470.45	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	86.01	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.396		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinqol	2535.00		NIST Webbook
tb	878.68	K	Joback Method
tc	1120.03	K	Joback Method
tf	548.39	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.83	J/molxK	878.68	Joback Method
cpg	666.87	J/molxK	918.91	Joback Method
cpg	676.66	J/molxK	959.13	Joback Method
cpg	685.23	J/molxK	999.36	Joback Method
cpg	692.61	J/molxK	1039.58	Joback Method
cpg	698.83	J/molxK	1079.81	Joback Method
cpg	703.93	J/molxK	1120.03	Joback Method
dvisc	0.0004633	Paxs	548.39	Joback Method
dvisc	0.0002816	Paxs	603.44	Joback Method

dvisc	0.0001861	Paxs	658.49	Joback Method
dvisc	0.0001310	Paxs	713.53	Joback Method
dvisc	0.0000970	Paxs	768.58	Joback Method
dvisc	0.0000748	Paxs	823.63	Joback Method
dvisc	0.0000596	Paxs	878.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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