3-(4-Chloro-2-methyl phenoxy)-1,2-propanediol-bis-(2,2-dichloropropio

Inchi: InChI=1S/C16H17Cl5O5/c1-9-6-10(17)4-5-12(9)24-7-11(26-14(23)16(3,20)21)8-25-13(22

InchiKey: AOINDYIVJHQCMT-UHFFFAOYSA-N

Formula: C16H17Cl5O5

SMILES: Cc1cc(Cl)ccc1OCC(COC(=O)C(C)(Cl)Cl)OC(=O)C(C)(Cl)Cl

Mol. weight [g/mol]: 466.57

CAS: 101292-50-6

Physical Properties

Property code	Value	Unit	Source
gf	-452.26	kJ/mol	Joback Method
hf	-883.28	kJ/mol	Joback Method
hfus	39.86	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.870		Crippen Method
mcvol	294.490	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
tb	957.37	K	Joback Method
tc	1195.40	K	Joback Method
tf	627.53	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.97	J/mol×K	957.37	Joback Method
cpg	797.92	J/mol×K	997.04	Joback Method
cpg	805.79	J/mol×K	1036.71	Joback Method
cpg	812.65	J/mol×K	1076.38	Joback Method
cpg	818.56	J/mol×K	1116.06	Joback Method
cpg	823.57	J/mol×K	1155.73	Joback Method
cpg	827.75	J/mol×K	1195.40	Joback Method
dvisc	0.0001564	Pa×s	627.53	Joback Method
dvisc	0.0000938	Pa×s	682.50	Joback Method

dvisc	0.0000607	Pa×s	737.48	Joback Method
dvisc	0.0000418	Pa×s	792.45	Joback Method
dvisc	0.0000301	Pa×s	847.42	Joback Method
dvisc	0.0000226	Pa×s	902.40	Joback Method
dvisc	0.0000176	Pa×s	957.37	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=C101292506&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume