2-Hydroxyethyl 2-(2,4,5-trichlorophenoxy)propanoate

Inchi: InChI=1S/C11H11Cl3O4/c1-6(11(16)17-3-2-15)18-10-5-8(13)7(12)4-9(10)14/h4-6,15H,2-

InchiKey: PDVSFMMXQVCJGE-UHFFFAOYSA-N

Formula: C11H11Cl3O4

SMILES: CC(Oc1cc(Cl)c(Cl)cc1Cl)C(=O)OCCO

Mol. weight [g/mol]: 313.56

CAS: 116402-64-3

Physical Properties

Property code	Value	Unit	Source
gf	-388.71	kJ/mol	Joback Method
hf	-650.00	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	85.35	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.950		Crippen Method
mcvol	197.990	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	795.44	K	Joback Method
tc	1006.75	K	Joback Method
tf	507.68	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.50	J/mol×K	795.44	Joback Method
cpg	524.88	J/mol×K	971.53	Joback Method
cpg	518.85	J/mol×K	936.31	Joback Method
cpg	512.09	J/mol×K	901.10	Joback Method
cpg	504.61	J/mol×K	865.88	Joback Method
cpg	496.41	J/mol×K	830.66	Joback Method
cpg	530.18	J/mol×K	1006.75	Joback Method
dvisc	0.0000215	Pa×s	795.44	Joback Method
dvisc	0.0000296	Pa×s	747.48	Joback Method

dvisc	0.0000427	Pa×s	699.52	Joback Method
dvisc	0.0000650	Pa×s	651.56	Joback Method
dvisc	0.0001057	Pa×s	603.60	Joback Method
dvisc	0.0001870	Pa×s	555.64	Joback Method
dvisc	0.0003683	Pa×s	507.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402643&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume