2-(3,4-Dichlorophenoxy)ethyl 2,2-dichloropropanoate

Inchi: InChI=1S/C11H10Cl4O3/c1-11(14,15)10(16)18-5-4-17-7-2-3-8(12)9(13)6-7/h2-3,6H,4-5H
InchiKey: QCMMKKFIKJOVEU-UHFFFAOYSA-N
Formula: C11H10Cl4O3
SMILES: CC(Cl)(Cl)C(=O)OCCOc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 332.01
CAS: 116402-59-6

Physical Properties

Property code	Value	Unit	Source
gf	-248.91	kJ/mol	Joback Method
hf	-505.51	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	4.109		Crippen Method
mcvol	204.360	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
tb	732.92	K	Joback Method
tc	967.10	K	Joback Method
tf	481.68	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.78	J/mol×K	732.92	Joback Method
cpg	511.88	J/mol×K	928.07	Joback Method
cpg	504.90	J/mol×K	889.04	Joback Method
cpg	497.12	J/mol×K	850.01	Joback Method
cpg	488.53	J/mol×K	810.98	Joback Method
cpg	479.09	J/mol×K	771.95	Joback Method
cpg	518.11	J/mol×K	967.10	Joback Method
dvisc	0.0000933	Pa×s	732.92	Joback Method
dvisc	0.0001165	Pa×s	691.05	Joback Method

dvisc	0.0001498	Pa×s	649.17	Joback Method
dvisc	0.0001994	Pa×s	607.30	Joback Method
dvisc	0.0002770	Pa×s	565.43	Joback Method
dvisc	0.0004054	Pa×s	523.55	Joback Method
dvisc	0.0006340	Pa×s	481.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402596&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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