

2-(2,4,5-Trichlorophenoxy)propyl 2,2-dichloropropanoate

Inchi:	InChI=1S/C12H11Cl5O3/c1-6(5-19-11(18)12(2,16)17)20-10-4-8(14)7(13)3-9(10)15/h3-4,
InchiKey:	FYNTVSDGWGTGOI-UHFFFAOYSA-N
Formula:	C12H11Cl5O3
SMILES:	CC(COC(=O)C(C)(Cl)Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	380.48
CAS:	100062-67-7

Physical Properties

Property code	Value	Unit	Source
gf	-264.49	kJ/mol	Joback Method
hf	-558.64	kJ/mol	Joback Method
hfus	33.73	kJ/mol	Joback Method
hvap	78.38	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.151		Crippen Method
mvol	230.690	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
tb	797.77	K	Joback Method
tc	1035.05	K	Joback Method
tf	520.39	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.24	J/molxK	797.77	Joback Method
cpg	549.07	J/molxK	837.32	Joback Method
cpg	557.98	J/molxK	876.86	Joback Method
cpg	566.00	J/molxK	916.41	Joback Method
cpg	573.16	J/molxK	955.96	Joback Method
cpg	579.48	J/molxK	995.51	Joback Method
cpg	585.01	J/molxK	1035.05	Joback Method
dvisc	0.0004566	Paxs	520.39	Joback Method
dvisc	0.0002877	Paxs	566.62	Joback Method

dvisc	0.0001944	Paxs	612.85	Joback Method
dvisc	0.0001388	Paxs	659.08	Joback Method
dvisc	0.0001035	Paxs	705.31	Joback Method
dvisc	0.0000801	Paxs	751.54	Joback Method
dvisc	0.0000638	Paxs	797.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100062677&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
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

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