

2-Methyl-2-(2,4,5-trichlorophenoxy)ethyl 2,2,3-trichloropropionate

Inchi:	InChI=1S/C12H10Cl6O3/c1-6(4-20-11(19)12(17,18)5-13)21-10-3-8(15)7(14)2-9(10)16/h2
InchiKey:	RZTWAUXNHFC SKX-UHFFFAOYSA-N
Formula:	C12H10Cl6O3
SMILES:	CC(COC(=O)C(Cl)(Cl)CCl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	414.92
CAS:	100136-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-276.42	kJ/mol	Joback Method
hf	-574.38	kJ/mol	Joback Method
hfus	37.93	kJ/mol	Joback Method
hvap	82.76	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.370		Crippen Method
mcvol	242.930	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
tb	835.20	K	Joback Method
tc	1074.78	K	Joback Method
tf	550.31	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.13	J/molxK	835.20	Joback Method
cpg	593.02	J/molxK	1034.85	Joback Method
cpg	587.70	J/molxK	994.92	Joback Method
cpg	581.59	J/molxK	954.99	Joback Method
cpg	574.65	J/molxK	915.06	Joback Method
cpg	566.84	J/molxK	875.13	Joback Method
cpg	597.57	J/molxK	1074.78	Joback Method
dvisc	0.0000540	Paxs	835.20	Joback Method
dvisc	0.0000676	Paxs	787.72	Joback Method

dvisc	0.0000871	Paxs	740.24	Joback Method
dvisc	0.0001162	Paxs	692.75	Joback Method
dvisc	0.0001618	Paxs	645.27	Joback Method
dvisc	0.0002375	Paxs	597.79	Joback Method
dvisc	0.0003724	Paxs	550.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100136116&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
mccvol:	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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