

2-(2,4,5-Trichlorophenoxy)ethyl 2,2,3-trichloropropanoate

Inchi:	InChI=1S/C11H8Cl6O3/c12-5-11(16,17)10(18)20-2-1-19-9-4-7(14)6(13)3-8(9)15/h3-4H,1
InchiKey:	MAYFADXVKRHMA-UHFFFAOYSA-N
Formula:	C11H8Cl6O3
SMILES:	O=C(OCCOc1cc(Cl)c(Cl)cc1Cl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	400.90
CAS:	99973-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-282.40	kJ/mol	Joback Method
hf	-548.46	kJ/mol	Joback Method
hfus	38.86	kJ/mol	Joback Method
hvap	80.92	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.982		Crippen Method
mcvol	228.840	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
tb	812.76	K	Joback Method
tc	1052.35	K	Joback Method
tf	554.04	K	Joback Method
vc	0.869	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.33	J/molxK	812.76	Joback Method
cpg	513.41	J/molxK	852.69	Joback Method
cpg	520.66	J/molxK	892.62	Joback Method
cpg	527.12	J/molxK	932.56	Joback Method
cpg	532.81	J/molxK	972.49	Joback Method
cpg	537.76	J/molxK	1012.42	Joback Method
cpg	542.00	J/molxK	1052.35	Joback Method
dvisc	0.0003808	Paxs	554.04	Joback Method
dvisc	0.0002581	Paxs	597.16	Joback Method

dvisc	0.0001843	Paxs	640.28	Joback Method
dvisc	0.0001374	Paxs	683.40	Joback Method
dvisc	0.0001060	Paxs	726.52	Joback Method
dvisc	0.0000842	Paxs	769.64	Joback Method
dvisc	0.0000685	Paxs	812.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99973918&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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