

2-(3,4-Dichlorophenoxy)-1-methylethyl 2,2-dichloropropanoate

Inchi:	InChI=1S/C12H12Cl4O3/c1-7(19-11(17)12(2,15)16)6-18-8-3-4-9(13)10(14)5-8/h3-5,7H,6
InchiKey:	KGLPCYVCDGKBJA-UHFFFAOYSA-N
Formula:	C12H12Cl4O3
SMILES:	CC(COc1ccc(Cl)c(Cl)c1)OC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	346.03
CAS:	116402-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-242.93	kJ/mol	Joback Method
hf	-531.43	kJ/mol	Joback Method
hfus	29.93	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.498		Crippen Method
mcvol	218.450	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
tb	755.36	K	Joback Method
tc	989.53	K	Joback Method
tf	477.95	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.51	J/molxK	755.36	Joback Method
cpg	531.57	J/molxK	794.39	Joback Method
cpg	541.68	J/molxK	833.42	Joback Method
cpg	550.87	J/molxK	872.44	Joback Method
cpg	559.18	J/molxK	911.47	Joback Method
cpg	566.64	J/molxK	950.50	Joback Method
cpg	573.27	J/molxK	989.53	Joback Method
dvisc	0.0006522	Paxs	477.95	Joback Method
dvisc	0.0003872	Paxs	524.18	Joback Method

dvisc	0.0002501	Paxs	570.42	Joback Method
dvisc	0.0001725	Paxs	616.65	Joback Method
dvisc	0.0001253	Paxs	662.89	Joback Method
dvisc	0.0000949	Paxs	709.12	Joback Method
dvisc	0.0000744	Paxs	755.36	Joback Method

Sources

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=C116402609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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