

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

Inchi:	InChI=1S/C11H9Cl5O3/c12-6-11(15,16)10(17)19-4-3-18-7-1-2-8(13)9(14)5-7/h1-2,5H,3-
InchiKey:	HGMQVASYZZSHJR-UHFFFAOYSA-N
Formula:	C11H9Cl5O3
SMILES:	O=C(OCCOc1ccc(Cl)c(Cl)c1)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	366.45
CAS:	99972-22-2

Physical Properties

Property code	Value	Unit	Source
gf	-260.84	kJ/mol	Joback Method
hf	-521.25	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	4.328		Crippen Method
mcvol	216.600	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
tb	770.35	K	Joback Method
tc	1006.93	K	Joback Method
tf	511.60	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.81	J/molxK	770.35	Joback Method
cpg	526.67	J/molxK	967.50	Joback Method
cpg	520.69	J/molxK	928.07	Joback Method
cpg	513.94	J/molxK	888.64	Joback Method
cpg	506.41	J/molxK	849.21	Joback Method
cpg	498.04	J/molxK	809.78	Joback Method
cpg	531.94	J/molxK	1006.93	Joback Method
dvisc	0.0000802	Paxs	770.35	Joback Method
dvisc	0.0000999	Paxs	727.23	Joback Method

dvisc	0.0001281	Paxs	684.10	Joback Method
dvisc	0.0001698	Paxs	640.98	Joback Method
dvisc	0.0002344	Paxs	597.85	Joback Method
dvisc	0.0003402	Paxs	554.73	Joback Method
dvisc	0.0005257	Paxs	511.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99972222&Units=SI

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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