

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

Inchi:	InChI=1S/C13H13Cl5O3/c14-8-13(17,18)12(19)21-6-2-1-5-20-11-4-3-9(15)7-10(11)16/h3
InchiKey:	BGPDOPQNJMHBI-XUHFFFAOYSA-N
Formula:	C13H13Cl5O3
SMILES:	O=C(OCCCCOc1ccc(Cl)cc1Cl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	394.51
CAS:	116402-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-244.00	kJ/mol	Joback Method
hf	-562.53	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.108		Crippen Method
mvol	244.780	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
tb	816.11	K	Joback Method
tc	1045.20	K	Joback Method
tf	534.14	K	Joback Method
vc	0.931	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.15	J/molxK	816.11	Joback Method
cpg	635.43	J/molxK	1007.01	Joback Method
cpg	628.64	J/molxK	968.83	Joback Method
cpg	621.06	J/molxK	930.65	Joback Method
cpg	612.64	J/molxK	892.47	Joback Method
cpg	603.35	J/molxK	854.29	Joback Method
cpg	641.47	J/molxK	1045.20	Joback Method
dvisc	0.0000593	Paxs	816.11	Joback Method
dvisc	0.0000745	Paxs	769.11	Joback Method

dvisc	0.0000964	Paxs	722.12	Joback Method
dvisc	0.0001294	Paxs	675.12	Joback Method
dvisc	0.0001815	Paxs	628.13	Joback Method
dvisc	0.0002690	Paxs	581.13	Joback Method
dvisc	0.0004270	Paxs	534.14	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=C116402632&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
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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