

2-(2,4,5-Trichlorophenoxy)ethyl trichloroacetate

Inchi:	InChI=1S/C10H6Cl6O3/c11-5-3-7(13)8(4-6(5)12)18-1-2-19-9(17)10(14,15)16/h3-4H,1-2H
InchiKey:	FFRUQSUMDFNBLG-UHFFFAOYSA-N
Formula:	C10H6Cl6O3
SMILES:	O=C(OCCOc1cc(Cl)c(Cl)cc1Cl)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	386.87
CAS:	25056-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-290.82	kJ/mol	Joback Method
hf	-527.82	kJ/mol	Joback Method
hfus	36.27	kJ/mol	Joback Method
hvap	78.70	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.939		Crippen Method
mvol	214.750	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	789.88	K	Joback Method
tc	1033.88	K	Joback Method
tf	542.77	K	Joback Method
vc	0.812	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.27	J/molxK	789.88	Joback Method
cpg	461.75	J/molxK	830.55	Joback Method
cpg	468.44	J/molxK	871.21	Joback Method
cpg	474.37	J/molxK	911.88	Joback Method
cpg	479.55	J/molxK	952.54	Joback Method
cpg	484.02	J/molxK	993.21	Joback Method
cpg	487.81	J/molxK	1033.88	Joback Method
dvisc	0.0004216	Paxs	542.77	Joback Method
dvisc	0.0002896	Paxs	583.95	Joback Method

dvisc	0.0002090	Paxs	625.14	Joback Method
dvisc	0.0001571	Paxs	666.33	Joback Method
dvisc	0.0001220	Paxs	707.51	Joback Method
dvisc	0.0000974	Paxs	748.69	Joback Method
dvisc	0.0000797	Paxs	789.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C25056706&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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