

2-[2-(2,4,5-Trichlorophenoxy)ethoxy]ethanol

Inchi:	InChI=1S/C10H11Cl3O3/c11-7-5-9(13)10(6-8(7)12)16-4-3-15-2-1-14/h5-6,14H,1-4H2
InchiKey:	YLGIDQAAEOZPLC-UHFFFAOYSA-N
Formula:	C10H11Cl3O3
SMILES:	OCCOCCOc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	285.55
CAS:	90920-28-8

Physical Properties

Property code	Value	Unit	Source
gf	-265.77	kJ/mol	Joback Method
hf	-511.50	kJ/mol	Joback Method
hfus	33.58	kJ/mol	Joback Method
hvap	76.77	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.035		Crippen Method
mcvol	182.330	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	719.13	K	Joback Method
tc	922.99	K	Joback Method
tf	461.48	K	Joback Method
vc	0.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.79	J/molxK	719.13	Joback Method
cpg	437.22	J/molxK	753.11	Joback Method
cpg	446.07	J/molxK	787.08	Joback Method
cpg	454.33	J/molxK	821.06	Joback Method
cpg	462.01	J/molxK	855.04	Joback Method
cpg	469.10	J/molxK	889.01	Joback Method
cpg	475.59	J/molxK	922.99	Joback Method
dvisc	0.0005265	Paxs	461.48	Joback Method
dvisc	0.0002706	Paxs	504.42	Joback Method

dvisc	0.0001543	Paxs	547.36	Joback Method
dvisc	0.0000955	Paxs	590.31	Joback Method
dvisc	0.0000631	Paxs	633.25	Joback Method
dvisc	0.0000439	Paxs	676.19	Joback Method
dvisc	0.0000319	Paxs	719.13	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=C90920288&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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