2-(2,4,5-Trichlorophenoxy)ethanol

Other names: Ethanol, 2-(2,4,5-trichlorophenoxy)-
Inchi: InChI=1S/C8H7Cl3O2/c9-5-3-7(11)8(4-6(5)10)13-2-1-12/h3-4,12H,1-2H2
InchiKey: ATKFMEGWDYLXBP-UHFFFAOYSA-N
Formula: C8H7Cl3O2
SMILES: OCCOc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 241.50
CAS: 2122-77-2

Physical Properties

Property code	Value	Unit	Source
gf	-177.61	kJ/mol	Joback Method
hf	-338.00	kJ/mol	Joback Method
hfus	27.22	kJ/mol	Joback Method
hvap	69.91	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.018		Crippen Method
mcvol	148.280	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	650.95	K	Joback Method
tc	862.24	K	Joback Method
tf	416.71	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.52	J/mol×K	650.95	Joback Method
cpg	343.21	J/mol×K	827.02	Joback Method
cpg	337.18	J/mol×K	791.81	Joback Method
cpg	330.70	J/mol×K	756.59	Joback Method
cpg	323.77	J/mol×K	721.38	Joback Method
cpg	316.37	J/mol×K	686.16	Joback Method
cpg	348.78	J/mol×K	862.24	Joback Method
dvisc	0.0000621	Pa×s	650.95	Joback Method

dvisc	0.0000859	Pa×s	611.91	Joback Method
dvisc	0.0001240	Pa×s	572.87	Joback Method
dvisc	0.0001889	Pa×s	533.83	Joback Method
dvisc	0.0003076	Pa×s	494.79	Joback Method
dvisc	0.0005446	Pa×s	455.75	Joback Method
dvisc	0.0010729	Pa×s	416.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2122772&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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