

2-(2,4,5-Trichlorophenoxy)-1-propanol

Inchi:	InChI=1S/C9H9Cl3O2/c1-5(4-13)14-9-3-7(11)6(10)2-8(9)12/h2-3,5,13H,4H2,1H3
InchiKey:	LYJSRGNLYMKMOP-UHFFFAOYSA-N
Formula:	C9H9Cl3O2
SMILES:	CC(CO)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	255.53

Physical Properties

Property code	Value	Unit	Source
gf	-171.63	kJ/mol	Joback Method
hf	-363.92	kJ/mol	Joback Method
hfus	26.28	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.406		Crippen Method
mcvol	162.370	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	673.39	K	Joback Method
tc	885.35	K	Joback Method
tf	412.98	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.31	J/molxK	673.39	Joback Method
cpg	365.22	J/molxK	708.72	Joback Method
cpg	373.59	J/molxK	744.04	Joback Method
cpg	381.42	J/molxK	779.37	Joback Method
cpg	388.71	J/molxK	814.70	Joback Method
cpg	395.48	J/molxK	850.03	Joback Method
cpg	401.73	J/molxK	885.35	Joback Method
dvisc	0.0012032	Paxs	412.98	Joback Method
dvisc	0.0005460	Paxs	456.38	Joback Method
dvisc	0.0002842	Paxs	499.78	Joback Method

dvisc	0.0001642	Paxs	543.18	Joback Method
dvisc	0.0001029	Paxs	586.59	Joback Method
dvisc	0.0000688	Paxs	629.99	Joback Method
dvisc	0.0000484	Paxs	673.39	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=B6001999&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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