

3-(2,4,5-Trichlorophenoxy)-1,2-propanediol-bis-2,2

Inchi:	InChI=1S/C15H11Cl9O5/c16-5-14(21,22)12(25)28-4-7(29-13(26)15(23,24)6-17)3-27-11-
InchiKey:	QWIBKUQOFSIULI-UHFFFAOYSA-N
Formula:	C15H11Cl9O5
SMILES:	O=C(OCC(COc1cc(Cl)c(Cl)cc1Cl)OC(=O)C(Cl)(Cl)CCl)C(Cl)(Cl)CCl
Mol. weight [g/mol]:	590.32
CAS:	100961-23-7

Physical Properties

Property code	Value	Unit	Source
gf	-518.03	kJ/mol	Joback Method
hf	-937.07	kJ/mol	Joback Method
hfus	53.66	kJ/mol	Joback Method
hvap	110.45	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.306		Crippen Method
mcvol	329.360	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
tb	1089.19	K	Joback Method
tc	1344.71	K	Joback Method
tf	748.46	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.94	J/molxK	1089.19	Joback Method
cpg	802.04	J/molxK	1302.12	Joback Method
cpg	800.86	J/molxK	1259.53	Joback Method
cpg	799.04	J/molxK	1216.95	Joback Method
cpg	796.49	J/molxK	1174.36	Joback Method
cpg	793.15	J/molxK	1131.78	Joback Method
cpg	802.65	J/molxK	1344.71	Joback Method
dvisc	0.0000091	Paxs	1089.19	Joback Method
dvisc	0.0000115	Paxs	1032.40	Joback Method

dvisc	0.0000148	Paxs	975.61	Joback Method
dvisc	0.0000197	Paxs	918.83	Joback Method
dvisc	0.0000272	Paxs	862.04	Joback Method
dvisc	0.0000394	Paxs	805.25	Joback Method
dvisc	0.0000604	Paxs	748.46	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=C100961237&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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