

2-(4-Chloro-o-toloxyl)ethyl alpha,alpha-dichloropropionate

Inchi:	InChI=1S/C12H13Cl3O3/c1-8-7-9(13)3-4-10(8)17-5-6-18-11(16)12(2,14)15/h3-4,7H,5-6H
InchiKey:	YXRNUAFSOKLXCL-UHFFFAOYSA-N
Formula:	C12H13Cl3O3
SMILES:	Cc1cc(Cl)ccc1OCCOC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	311.59
CAS:	100120-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-228.56	kJ/mol	Joback Method
hf	-510.41	kJ/mol	Joback Method
hfus	29.25	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.764		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	718.37	K	Joback Method
tc	945.73	K	Joback Method
tf	463.03	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.80	J/molxK	718.37	Joback Method
cpg	509.78	J/molxK	756.26	Joback Method
cpg	520.84	J/molxK	794.16	Joback Method
cpg	531.01	J/molxK	832.05	Joback Method
cpg	540.32	J/molxK	869.95	Joback Method
cpg	548.80	J/molxK	907.84	Joback Method
cpg	556.47	J/molxK	945.73	Joback Method
dvisc	0.0006938	Paxs	463.03	Joback Method
dvisc	0.0004312	Paxs	505.59	Joback Method

dvisc	0.0002886	Paxs	548.14	Joback Method
dvisc	0.0002046	Paxs	590.70	Joback Method
dvisc	0.0001519	Paxs	633.26	Joback Method
dvisc	0.0001171	Paxs	675.81	Joback Method
dvisc	0.0000931	Paxs	718.37	Joback Method

Sources

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=C100120216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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