

Alpha,alpha-dichloropropionic acid, 2-(2,4-dibromophenoxy) ethyl ester

Inchi:	InChI=1S/C11H10Br2Cl2O3/c1-11(14,15)10(16)18-5-4-17-9-3-2-7(12)6-8(9)13/h2-3,6H,4
InchiKey:	RJZAJEHYXYGMOO-UHFFFAOYSA-N
Formula:	C11H10Br2Cl2O3
SMILES:	CC(Cl)(Cl)C(=O)OCCOc1ccc(Br)cc1Br
Mol. weight [g/mol]:	420.91
CAS:	99983-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-196.41	kJ/mol	Joback Method
hf	-421.37	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.327		Crippen Method
mcvol	214.880	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
tb	790.38	K	Joback Method
tc	1039.23	K	Joback Method
tf	541.44	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.96	J/molxK	790.38	Joback Method
cpg	494.39	J/molxK	831.86	Joback Method
cpg	502.95	J/molxK	873.33	Joback Method
cpg	510.72	J/molxK	914.81	Joback Method
cpg	517.74	J/molxK	956.28	Joback Method
cpg	524.07	J/molxK	997.76	Joback Method
cpg	529.77	J/molxK	1039.23	Joback Method
dvisc	0.0004213	Paxs	541.44	Joback Method
dvisc	0.0002870	Paxs	582.93	Joback Method

dvisc	0.0002057	Paxs	624.42	Joback Method
dvisc	0.0001537	Paxs	665.91	Joback Method
dvisc	0.0001189	Paxs	707.40	Joback Method
dvisc	0.0000946	Paxs	748.89	Joback Method
dvisc	0.0000771	Paxs	790.38	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=C99983489&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
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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