Chloropropylate

Other names:

1-Methylethyl 4-chloro-«alpha»-(4-chlorophenyl)-«alpha»-hydroxybenzeneacetate

1-Methylethyl 4-chloro-Â«alphaÂ»-(4-chlorophenyl)-Â«alphaÂ»-hydroxybenzeneacetate

Acaralate

Benzeneacetic acid, 4-chloro-«alpha»-(4-chlorophenyl)-«alpha»-hydroxy-, 1-methylethyl ester

Benzeneacetic acid, 4-chloro-Â«alphaÂ»-(4-chlorophenyl)-Â«alphaÂ»-hydroxy-, 1-methylethyl ester

Benzilic acid, 4,4'-dichloro-, isopropyl ester

Chlormite

Chlorpropylat

Chlorpropylate

ENT 26,999

G 24,163

GEIGY 24163

Gesakur

Isopropyl 4,4'-Dichlorobenzilate

Isopropylester kyseliny 4,4'-dichlorbenzilove

Rospan

Rospin

Rospine

propan-2-yl 2,2-bis(4-chlorophenyl)-2-hydroxyacetate

Inchi: InChI=1S/C17H16Cl2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6

InchiKey: AXGUBXVWZBFQGA-UHFFFAOYSA-N

Formula: C17H16Cl2O3

SMILES: CC(C)OC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1

Mol. weight [g/mol]: 339.21

CAS: 5836-10-2

Physical Properties

Property code	Value	Unit	Source
gf	-96.38	kJ/mol	Joback Method
hf	-386.63	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-4.53		Aqueous Solubility Prediction Method
log10ws	-4.53		Estimated Solubility Method
logp	4.181		Crippen Method

mcvol	240.660	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
ripol	3337.00		NIST Webbook
tb	891.34	K	Joback Method
tc	1125.88	K	Joback Method
tf	345.00 ± 0.20	K	NIST Webbook
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.52	J/mol×K	891.34	Joback Method
cpg	681.22	J/mol×K	930.43	Joback Method
cpg	690.98	J/mol×K	969.52	Joback Method
cpg	699.87	J/mol×K	1008.61	Joback Method
cpg	707.97	J/mol×K	1047.70	Joback Method
cpg	715.37	J/mol×K	1086.79	Joback Method
cpg	722.15	J/mol×K	1125.88	Joback Method
dvisc	0.0002718	Pa×s	539.47	Joback Method
dvisc	0.0001181	Pa×s	598.12	Joback Method
dvisc	0.0000596	Pa×s	656.76	Joback Method
dvisc	0.0000336	Pa×s	715.40	Joback Method
dvisc	0.0000207	Pa×s	774.05	Joback Method
dvisc	0.0000136	Pa×s	832.69	Joback Method
dvisc	0.0000095	Pa×s	891.34	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5836102&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume