Chlorobenzilate

Other names:	Benzeneacetic acid, 4-chloro-«alpha»-(4-chlorophenyl)-«alpha»-hydroxy-, ethyl ester Benzilic acid, 4,4'-dichloro-, ethyl ester Acar Acaraben Akar Akar 338 Benzilan Chlorbenzilat Chlorbenzylate Compound 338 Ethyl 4,4'-dichlorobenzilate Folbex G 23992 G 338 Geigy 338 4,4'-Dichlorobenzilic acid ethyl ester Chlorobenzylate Ethyl ester of 4,4'-dichlorobenzilic acid Ethyl p,p'-dichlorobenzilate Ethyl 4,4'-dichlorodiphenyl glycollate Ethyl 4,4'-dichlorophenyl glycollate Ethyl-2-hydroxy-2,2-bis(4-chlorophenyl)acetate ENT 18,596 Kop-Mite NCI-C00408 4,4'-Dichlorbenzilsaeureaethylester Acaraben 4E Akar 50 Benz-O-chlor Chlorbenzilate Ethyl 4-chloro-«alpha»-(4-chlorophenyl)-«alpha»-hydroxybenzeneacetate Ethylester kyseliny 4,4-dichlorbenzilove Folbex smoke-strips NCI-C60413 Rcra waste number U038
Inchi:	InChI=1S/C16H14Cl2O3/c1-2-21-15(19)16(20,11-3-7-13(17)8-4-11)12-5-9-14(18)10-6-12
InchiKey:	RAPBNVDSDCTNRC-UHFFFAOYSA-N
Formula:	C16H14Cl2O3
SMILES:	CCOC(=O)C(O)(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	325.19

CAS: 510-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-102.36	kJ/mol	Joback Method
hf	-360.71	kJ/mol	Joback Method
hfus	32.35	kJ/mol	Joback Method
hvap	90.40	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.792		Crippen Method
mcvol	226.570	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	372.66		NIST Webbook
rinpol	372.66		NIST Webbook
rinpol	2204.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2261.00		NIST Webbook
rinpol	371.32		NIST Webbook
ripol	3230.00		NIST Webbook
tb	868.90	K	Joback Method
tc	1102.84	K	Joback Method
tf	312.19 ± 0.20	K	NIST Webbook
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.28	J/mol×K	1102.84	Joback Method
cpg	657.80	J/mol×K	1063.85	Joback Method
cpg	650.72	J/mol×K	1024.86	Joback Method
cpg	642.95	J/mol×K	985.87	Joback Method
cpg	634.44	J/mol×K	946.88	Joback Method
cpg	625.08	J/mol×K	907.89	Joback Method
cpg	614.82	J/mol×K	868.90	Joback Method
dvisc	0.0002689	Pa×s	543.20	Joback Method
dvisc	0.0000125	Pa×s	868.90	Joback Method
dvisc	0.0000175	Pa×s	814.62	Joback Method

dvisc	0.0000259	Pa×s	760.33	Joback Method
dvisc	0.0000406	Pa×s	706.05	Joback Method
dvisc	0.0000687	Pa×s	651.77	Joback Method
dvisc	0.0001277	Pa×s	597.48	Joback Method
hfust	23.48	kJ/mol	310.40	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C510156&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
hfust:	Enthalpy of fusion at a given temperature
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