Bromopropylate

Other names:	Benzeneacetic acid, 4-bromo-«alpha»-(4-bromophenyl)-«alpha»-hydroxy-, 1-methylethyl ester Benzilic acid, 4,4'-dibromo-, isopropyl ester Acarol Geigy 19851 GS 19851 Isopropyl dibromobenzilate Isopropyl 4,4'-dibromobenzilate Neoron Bromobropylate Phenisobromolate Folbex VA
Inchi:	InChI=1S/C17H16Br2O3/c1-11(2)22-16(20)17(21,12-3-7-14(18)8-4-12)13-5-9-15(19)10-6
InchiKey:	FOANIXZHAMJWOI-UHFFFAOYSA-N
Formula:	C17H16Br2O3
SMILES:	CC(C)OC(=O)C(O)(c1ccc(Br)cc1)c1ccc(Br)cc1
Mol. weight [g/mol]:	428.12
CAS:	18181-80-1

Physical Properties

Property code	Value	Unit	Source
gf	-43.88	kJ/mol	Joback Method
hf	-302.49	kJ/mol	Joback Method
hfus	33.60	kJ/mol	Joback Method
hvap	96.33	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	4.399		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
tb	948.80	K	Joback Method
tc	1195.82	K	Joback Method
tf	349.12 ± 0.20	K	NIST Webbook
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.66	J/mol×K	1195.82	Joback Method
cpg	731.19	J/mol×K	1154.65	Joback Method
cpg	723.43	J/mol×K	1113.48	Joback Method
cpg	715.26	J/mol×K	1072.31	Joback Method
cpg	706.57	J/mol×K	1031.14	Joback Method
cpg	697.24	J/mol×K	989.97	Joback Method
cpg	687.16	J/mol×K	948.80	Joback Method
dvisc	0.0001371	Pa×s	599.23	Joback Method
dvisc	0.0000071	Pa×s	948.80	Joback Method
dvisc	0.0000099	Pa×s	890.54	Joback Method
dvisc	0.0000145	Pa×s	832.28	Joback Method
dvisc	0.0000224	Pa×s	774.01	Joback Method
dvisc	0.0000371	Pa×s	715.75	Joback Method
dvisc	0.0000673	Pa×s	657.49	Joback Method
hfust	24.55	kJ/mol	348.10	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=C18181801&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume