Benzoic acid, 3-chloro-, anhydride

Other names: 3-Chlorobenzoic anhydride
Inchi: InChI=1S/C14H8Cl2O3/c15-11-5-1-3-9(7-11)13(17)19-14(18)10-4-2-6-12(16)8-10/h1-8H
InchiKey: NIHKFGMYMWGERR-UHFFFAOYSA-N
Formula: C14H8Cl2O3
SMILES: O=C(OC(=O)c1cccc(Cl)c1)c1cccc(Cl)c1
Mol. weight [g/mol]: 295.12
CAS: 30070-63-4

Physical Properties

Property code	Value	Unit	Source
gf	-114.14	kJ/mol	Joback Method
hf	-271.03	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	3.991		Crippen Method
mcvol	194.090	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	2269.70		NIST Webbook
tb	788.06	K	Joback Method
tc	1041.94	K	Joback Method
tf	507.35	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.63	J/mol×K	788.06	Joback Method
cpg	511.50	J/mol×K	999.63	Joback Method
cpg	505.12	J/mol×K	957.31	Joback Method
cpg	497.80	J/mol×K	915.00	Joback Method
cpg	489.47	J/mol×K	872.69	Joback Method
cpg	480.10	J/mol×K	830.37	Joback Method
cpg	516.96	J/mol×K	1041.94	Joback Method

dvisc	0.0001284	Pa×s	788.06	Joback Method
dvisc	0.0001574	Pa×s	741.27	Joback Method
dvisc	0.0001985	Pa×s	694.49	Joback Method
dvisc	0.0002588	Pa×s	647.70	Joback Method
dvisc	0.0003516	Pa×s	600.92	Joback Method
dvisc	0.0005031	Pa×s	554.13	Joback Method
dvisc	0.0007691	Pa×s	507.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30070634&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume