

2-Chlorobenzoic acid, isopropyl ester

Other names:	Benzoic acid, 2-chloro, 1-methylethyl ester
Inchi:	InChI=1S/C10H11ClO2/c1-7(2)13-10(12)8-5-3-4-6-9(8)11/h3-7H,1-2H3
InchiKey:	ZQVYNQNVFVRHMT-UHFFFAOYSA-N
Formula:	C10H11ClO2
SMILES:	CC(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	198.65
CAS:	942-14-3

Physical Properties

Property code	Value	Unit	Source
gf	-112.19	kJ/mol	Joback Method
hf	-290.49	kJ/mol	Joback Method
hfus	18.77	kJ/mol	Joback Method
hvap	53.95	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.905		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1345.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1352.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1936.00		NIST Webbook
tb	573.14	K	Joback Method
tc	796.07	K	Joback Method
tf	328.48	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.36	J/mol×K	573.14	Joback Method
cpg	382.87	J/mol×K	758.92	Joback Method
cpg	373.05	J/mol×K	721.76	Joback Method
cpg	362.51	J/mol×K	684.61	Joback Method
cpg	351.23	J/mol×K	647.45	Joback Method
cpg	339.19	J/mol×K	610.30	Joback Method
cpg	391.97	J/mol×K	796.07	Joback Method
dvisc	0.0001966	Pa×s	573.14	Joback Method
dvisc	0.0002504	Pa×s	532.36	Joback Method
dvisc	0.0003321	Pa×s	491.59	Joback Method
dvisc	0.0004634	Pa×s	450.81	Joback Method
dvisc	0.0006911	Pa×s	410.03	Joback Method
dvisc	0.0011257	Pa×s	369.26	Joback Method
dvisc	0.0020698	Pa×s	328.48	Joback Method

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=C942143&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
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

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