

3-Chlorobenzoic acid, 4-chloro-2-methylphenyl ester

Inchi:	InChI=1S/C14H10Cl2O2/c1-9-7-12(16)5-6-13(9)18-14(17)10-3-2-4-11(15)8-10/h2-8H,1H
InchiKey:	BHLWDJNYZGNVBZ-UHFFFAOYSA-N
Formula:	C14H10Cl2O2
SMILES:	Cc1cc(Cl)ccc1OC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	281.13

Physical Properties

Property code	Value	Unit	Source
gf	5.15	kJ/mol	Joback Method
hf	-169.92	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.521		Crippen Method
mcvol	192.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinsol	2155.00		NIST Webbook
tb	739.17	K	Joback Method
tc	989.16	K	Joback Method
tf	469.94	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.79	J/molxK	739.17	Joback Method
cpg	510.53	J/molxK	947.50	Joback Method
cpg	502.38	J/molxK	905.83	Joback Method
cpg	493.27	J/molxK	864.17	Joback Method
cpg	483.16	J/molxK	822.50	Joback Method
cpg	472.01	J/molxK	780.84	Joback Method
cpg	517.76	J/molxK	989.16	Joback Method
dvisc	0.0001294	Paxs	739.17	Joback Method
dvisc	0.0001576	Paxs	694.30	Joback Method

dvisc	0.0001972	Paxs	649.43	Joback Method
dvisc	0.0002551	Paxs	604.56	Joback Method
dvisc	0.0003439	Paxs	559.68	Joback Method
dvisc	0.0004884	Paxs	514.81	Joback Method
dvisc	0.0007416	Paxs	469.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357399&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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