

3-Chlorobenzoic acid, 3,4-dimethylphenyl ester

Inchi:	InChI=1S/C15H13ClO2/c1-10-6-7-14(8-11(10)2)18-15(17)12-4-3-5-13(16)9-12/h3-9H,1-2
InchiKey:	PLYGAVCVUAMEMN-UHFFFAOYSA-N
Formula:	C15H13ClO2
SMILES:	Cc1ccc(OC(=O)c2cccc(Cl)c2)cc1C
Mol. weight [g/mol]:	260.72

Physical Properties

Property code	Value	Unit	Source
gf	25.50	kJ/mol	Joback Method
hf	-174.82	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.176		Crippen Method
mcvol	194.370	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpola	2144.00		NIST Webbook
tb	724.62	K	Joback Method
tc	967.25	K	Joback Method
tf	451.29	K	Joback Method
vc	0.733	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.64	J/molxK	724.62	Joback Method
cpg	502.61	J/molxK	765.06	Joback Method
cpg	515.45	J/molxK	805.50	Joback Method
cpg	527.22	J/molxK	845.94	Joback Method
cpg	537.95	J/molxK	886.37	Joback Method
cpg	547.67	J/molxK	926.81	Joback Method
cpg	556.42	J/molxK	967.25	Joback Method
dvisc	0.0007771	Paxs	451.29	Joback Method
dvisc	0.0004995	Paxs	496.85	Joback Method

dvisc	0.0003458	Paxs	542.40	Joback Method
dvisc	0.0002534	Paxs	587.96	Joback Method
dvisc	0.0001942	Paxs	633.51	Joback Method
dvisc	0.0001543	Paxs	679.07	Joback Method
dvisc	0.0001261	Paxs	724.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357398&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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