2-Chlorobenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H13ClO2/c1-10-7-11(2)9-12(8-10)18-15(17)13-5-3-4-6-14(13)16/h3-9H,1-2

InchiKey: HHSLGRLKQCSCBW-UHFFFAOYSA-N

Formula: C15H13ClO2

SMILES: Cc1cc(C)cc(OC(=O)c2ccccc2Cl)c1

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
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	724.62	K	Joback Method
tc	967.25	K	Joback Method
tf	451.29	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.64	J/mol×K	724.62	Joback Method
cpg	502.61	J/mol×K	765.06	Joback Method
cpg	515.45	J/mol×K	805.50	Joback Method
cpg	527.22	J/mol×K	845.94	Joback Method
cpg	537.95	J/mol×K	886.37	Joback Method
cpg	547.67	J/mol×K	926.81	Joback Method
cpg	556.42	J/mol×K	967.25	Joback Method
dvisc	0.0007771	Pa×s	451.29	Joback Method

dvisc	0.0004995	Pa×s	496.85	Joback Method
dvisc	0.0003458	Pa×s	542.40	Joback Method
dvisc	0.0002534	Pa×s	587.96	Joback Method
dvisc	0.0001942	Pa×s	633.51	Joback Method
dvisc	0.0001543	Pa×s	679.07	Joback Method
dvisc	0.0001261	Pa×s	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=U307816&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