3-Chlorobenzoic acid, 4-isopropylphenyl ester

Inchi: InChI=1S/C16H15ClO2/c1-11(2)12-6-8-15(9-7-12)19-16(18)13-4-3-5-14(17)10-13/h3-11H
InchiKey: MIEAXDYYVFWBLV-UHFFFAOYSA-N
Formula: C16H15ClO2
SMILES: CC(C)c1ccc(OC(=O)c2cccc(Cl)c2)cc1
Mol. weight [g/mol]: 274.74

Physical Properties

Property code	Value	Unit	Source
gf	41.11	kJ/mol	Joback Method
hf	-189.27	kJ/mol	Joback Method
hfus	27.96	kJ/mol	Joback Method
hvap	70.24	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.683		Crippen Method
mcvol	208.460	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2168.00		NIST Webbook
tb	742.08	K	Joback Method
tc	983.66	K	Joback Method
tf	435.04	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.15	J/mol×K	742.08	Joback Method
cpg	605.35	J/mol×K	943.40	Joback Method
cpg	595.15	J/mol×K	903.13	Joback Method
cpg	583.88	J/mol×K	862.87	Joback Method
cpg	571.48	J/mol×K	822.61	Joback Method
cpg	557.92	J/mol×K	782.34	Joback Method
cpg	614.53	J/mol×K	983.66	Joback Method
dvisc	0.0001034	Pa×s	742.08	Joback Method
dvisc	0.0001309	Pa×s	690.91	Joback Method

dvisc	0.0001720	Pa×s	639.73	Joback Method
dvisc	0.0002370	Pa×s	588.56	Joback Method
dvisc	0.0003471	Pa×s	537.39	Joback Method
dvisc	0.0005509	Pa×s	486.21	Joback Method
dvisc	0.0009748	Pa×s	435.04	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=U357400&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume