

2-Chlorobenzoic acid, 4-tolyl ester

Inchi:	InChI=1S/C14H11ClO2/c1-10-6-8-11(9-7-10)17-14(16)12-4-2-3-5-13(12)15/h2-9H,1H3
InchiKey:	XLJNELFCIDKGTK-UHFFFAOYSA-N
Formula:	C14H11ClO2
SMILES:	<chem>Cc1ccc(OC(=O)c2ccccc2Cl)cc1</chem>
Mol. weight [g/mol]:	246.69
CAS:	6280-48-4

Physical Properties

Property code	Value	Unit	Source
gf	26.71	kJ/mol	Joback Method
hf	-142.71	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.868		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
tb	696.76	K	Joback Method
tc	943.81	K	Joback Method
tf	427.50	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.48	J/molxK	696.76	Joback Method
cpg	452.11	J/molxK	737.94	Joback Method
cpg	464.61	J/molxK	779.11	Joback Method
cpg	476.03	J/molxK	820.29	Joback Method
cpg	486.41	J/molxK	861.46	Joback Method
cpg	495.79	J/molxK	902.64	Joback Method
cpg	504.22	J/molxK	943.81	Joback Method
dvisc	0.0009660	Paxs	427.50	Joback Method
dvisc	0.0006014	Paxs	472.38	Joback Method

dvisc	0.0004065	Paxs	517.25	Joback Method
dvisc	0.0002925	Paxs	562.13	Joback Method
dvisc	0.0002210	Paxs	607.01	Joback Method
dvisc	0.0001735	Paxs	651.88	Joback Method
dvisc	0.0001405	Paxs	696.76	Joback Method

Sources

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=C6280484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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