3-Chlorobenzoic acid, 2-methylbutyl ester

Inchi: InChI=1S/C12H15ClO2/c1-3-9(2)8-15-12(14)10-5-4-6-11(13)7-10/h4-7,9H,3,8H2,1-2H3
InchiKey: HOQMVZSERAOHEF-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CCC(C)COC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-95.35	kJ/mol	Joback Method
hf	-331.77	kJ/mol	Joback Method
hfus	23.95	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.543		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1617.00		NIST Webbook
rinpol	1617.00		NIST Webbook
tb	618.90	K	Joback Method
tc	834.03	K	Joback Method
tf	351.02	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.78	J/mol×K	618.90	Joback Method
cpg	485.09	J/mol×K	798.18	Joback Method
cpg	474.07	J/mol×K	762.32	Joback Method
cpg	462.25	J/mol×K	726.47	Joback Method
cpg	449.61	J/mol×K	690.61	Joback Method
cpg	436.13	J/mol×K	654.76	Joback Method
cpg	495.33	J/mol×K	834.03	Joback Method
dvisc	0.0001617	Pa×s	618.90	Joback Method

dvisc	0.0002079	Pa×s	574.25	Joback Method
dvisc	0.0002788	Pa×s	529.61	Joback Method
dvisc	0.0003947	Pa×s	484.96	Joback Method
dvisc	0.0005996	Pa×s	440.31	Joback Method
dvisc	0.0010010	Pa×s	395.67	Joback Method
dvisc	0.0019039	Pa×s	351.02	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=U357394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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