2-Chlorobenzoic acid, 3-methylbutyl-2 ester

Other names: Benzoic acid, 2-chloro, 1,2-dimethylpropyl ester
Inchi: InChI=1S/C12H15ClO2/c1-8(2)9(3)15-12(14)10-6-4-5-7-11(10)13/h4-9H,1-3H3
InchiKey: GULZYXNRPUDADC-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CC(C)C(C)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-97.79	kJ/mol	Joback Method
hf	-337.05	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.541		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1521.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1529.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2084.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2098.00		NIST Webbook
ripol	2084.00		NIST Webbook
tb	618.46	K	Joback Method
tc	838.01	K	Joback Method
tf	336.02	K	Joback Method

vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.24	J/mol×K	618.46	Joback Method
cpg	436.93	J/mol×K	655.05	Joback Method
cpg	450.70	J/mol×K	691.64	Joback Method
cpg	463.59	J/mol×K	728.23	Joback Method
cpg	475.62	J/mol×K	764.82	Joback Method
cpg	486.79	J/mol×K	801.42	Joback Method
cpg	497.15	J/mol×K	838.01	Joback Method
dvisc	0.0024032	Pa×s	336.02	Joback Method
dvisc	0.0011407	Pa×s	383.09	Joback Method
dvisc	0.0006373	Pa×s	430.17	Joback Method
dvisc	0.0003994	Pa×s	477.24	Joback Method
dvisc	0.0002722	Pa×s	524.31	Joback Method
dvisc	0.0001976	Pa×s	571.39	Joback Method
dvisc	0.0001507	Pa×s	618.46	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=U360519&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume