Benzoic acid, 4-chloro, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C12H15ClO2/c1-8(2)9(3)15-12(14)10-4-6-11(13)7-5-10/h4-9H,1-3H3
InchiKey: OMYRCAJCAGZMSM-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CC(C)C(C)OC(=O)c1ccc(Cl)cc1
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	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1535.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2030.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2030.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R117025&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume