4-Chlorobenzoic acid, 3-methylbutyl ester

Other names: Benzoic acid, 4-chloro, 3-methylbutyl ester
Inchi: InChI=1S/C12H15ClO2/c1-9(2)7-8-15-12(14)10-3-5-11(13)6-4-10/h3-6,9H,7-8H2,1-2H3
InchiKey: YBRVJNBUZZRJDV-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: CC(C)CCOC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 226.70
CAS: 6942-75-2

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	1583.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1573.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1574.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2122.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2129.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2107.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6942752&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

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