4-Chlorobutyric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C12H15ClO2/c1-9-6-10(2)8-11(7-9)15-12(14)4-3-5-13/h6-8H,3-5H2,1-2H3
InchiKey: BWWVMEDTGZFRCA-UHFFFAOYSA-N
Formula: C12H15ClO2
SMILES: Cc1cc(C)cc(OC(=O)CCCCl)c1
Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-102.54	kJ/mol	Joback Method
hf	-337.96	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.228		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	624.32	K	Joback Method
tc	836.12	K	Joback Method
tf	378.54	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.60	J/mol×K	624.32	Joback Method
cpg	481.99	J/mol×K	800.82	Joback Method
cpg	471.22	J/mol×K	765.52	Joback Method
cpg	459.71	J/mol×K	730.22	Joback Method
cpg	447.44	J/mol×K	694.92	Joback Method
cpg	434.41	J/mol×K	659.62	Joback Method

cpg	492.04	J/mol×K	836.12	Joback Method
dvisc	0.0001712	Pa×s	624.32	Joback Method
dvisc	0.0002123	Pa×s	583.36	Joback Method
dvisc	0.0002718	Pa×s	542.39	Joback Method
dvisc	0.0003625	Pa×s	501.43	Joback Method
dvisc	0.0005088	Pa×s	460.47	Joback Method
dvisc	0.0007630	Pa×s	419.50	Joback Method
dvisc	0.0012490	Pa×s	378.54	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=U357772&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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