5-Chlorovaleric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C13H17ClO2/c1-10-7-11(2)9-12(8-10)16-13(15)5-3-4-6-14/h7-9H,3-6H2,1-2H3
InchiKey: ZZLQVNHJJPBAPS-UHFFFAOYSA-N
Formula: C13H17ClO2
SMILES: Cc1cc(C)cc(OC(=O)CCCCCl)c1
Mol. weight [g/mol]: 240.73

Physical Properties

Property code	Value	Unit	Source
gf	-94.12	kJ/mol	Joback Method
hf	-358.60	kJ/mol	Joback Method
hfus	29.67	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.618		Crippen Method
mcvol	189.950	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
tb	647.20	K	Joback Method
tc	855.70	K	Joback Method
tf	389.81	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.66	J/mol×K	647.20	Joback Method
cpg	485.09	J/mol×K	681.95	Joback Method
cpg	498.71	J/mol×K	716.70	Joback Method
cpg	511.53	J/mol×K	751.45	Joback Method
cpg	523.56	J/mol×K	786.20	Joback Method
cpg	534.81	J/mol×K	820.95	Joback Method
cpg	545.31	J/mol×K	855.70	Joback Method
dvisc	0.0011960	Pa×s	389.81	Joback Method

dvisc	0.0007183	Pa×s	432.71	Joback Method
dvisc	0.0004729	Pa×s	475.61	Joback Method
dvisc	0.0003337	Pa×s	518.50	Joback Method
dvisc	0.0002483	Pa×s	561.40	Joback Method
dvisc	0.0001927	Pa×s	604.30	Joback Method
dvisc	0.0001547	Pa×s	647.20	Joback Method

Sources

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=U307976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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