5-Chlorovaleric acid, 3-methylphenyl ester

Inchi: InChI=1S/C12H15ClO2/c1-10-5-4-6-11(9-10)15-12(14)7-2-3-8-13/h4-6,9H,2-3,7-8H2,1H3

InchiKey: RDYAPVUPQWREBE-UHFFFAOYSA-N

Formula: C12H15ClO2

SMILES: Cc1cccc(OC(=O)CCCCCl)c1

Mol. weight [g/mol]: 226.70

Physical Properties

Property code	Value	Unit	Source
gf	-92.91	kJ/mol	Joback Method
hf	-326.49	kJ/mol	Joback Method
hfus	27.47	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.310		Crippen Method
mcvol	175.860	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1695.00		NIST Webbook
tb	619.34	K	Joback Method
tc	830.22	K	Joback Method
tf	366.02	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.33	J/mol×K	619.34	Joback Method
cpg	483.41	J/mol×K	795.07	Joback Method
cpg	472.56	J/mol×K	759.93	Joback Method
cpg	460.94	J/mol×K	724.78	Joback Method
cpg	448.54	J/mol×K	689.63	Joback Method
cpg	435.34	J/mol×K	654.49	Joback Method
cpg	493.53	J/mol×K	830.22	Joback Method
dvisc	0.0001735	Pa×s	619.34	Joback Method
dvisc	0.0002188	Pa×s	577.12	Joback Method

dvisc	0.0002861	Pa×s	534.90	Joback Method
dvisc	0.0003918	Pa×s	492.68	Joback Method
dvisc	0.0005690	Pa×s	450.46	Joback Method
dvisc	0.0008929	Pa×s	408.24	Joback Method
dvisc	0.0015544	Pa×s	366.02	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=U307974&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