Pentanoic acid, 5-chloro-, ethyl ester

Other names: 5-Chlorovaleric acid, ethyl ester
Inchi: InChI=1S/C7H13ClO2/c1-2-10-7(9)5-3-4-6-8/h2-6H2,1H3
InchiKey: JHPBGAORCOXWNO-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCOC(=O)CCCCCl
Mol. weight [g/mol]: 164.63
CAS: 2323-81-1

Physical Properties

Property code	Value	Unit	Source
gf	-237.79	kJ/mol	Joback Method
hf	-448.35	kJ/mol	Joback Method
hfus	20.87	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.959		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
rinpol	1145.30		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1670.00		NIST Webbook
tb	473.28	K	Joback Method
tc	655.90	K	Joback Method
tf	270.73	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.22	J/mol×K	473.28	Joback Method
cpg	315.13	J/mol×K	625.46	Joback Method
cpg	305.96	J/mol×K	595.03	Joback Method
cpg	296.38	J/mol×K	564.59	Joback Method
cpg	286.40	J/mol×K	534.15	Joback Method

cpg	276.01	J/mol×K	503.72	Joback Method
cpg	323.90	J/mol×K	655.90	Joback Method
dvisc	0.0002820	Pa×s	473.28	Joback Method
dvisc	0.0003603	Pa×s	439.52	Joback Method
dvisc	0.0004794	Pa×s	405.76	Joback Method
dvisc	0.0006719	Pa×s	372.00	Joback Method
dvisc	0.0010072	Pa×s	338.25	Joback Method
dvisc	0.0016518	Pa×s	304.49	Joback Method
dvisc	0.0030645	Pa×s	270.73	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=C2323811&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: