Chloromethyl pentanoate

Other names: Pentanoic acid, chloromethyl ester
Inchi: InChI=1S/C6H11ClO2/c1-2-3-4-6(8)9-5-7/h2-5H2,1H3
InchiKey: ZYDSTVMBNBPPLQ-UHFFFAOYSA-N
Formula: C6H11ClO2
SMILES: CCCCC(=O)OCCl
Mol. weight [g/mol]: 150.60
CAS: 77877-94-2

Physical Properties

Property code	Value	Unit	Source
gf	-246.21	kJ/mol	Joback Method
hf	-427.71	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	42.49	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.916		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	953.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1374.00		NIST Webbook
tb	450.40	K	Joback Method
tc	634.77	K	Joback Method
tf	259.46	K	Joback Method
vc	0.445	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/mol×K	450.40	Joback Method
cpg	234.51	J/mol×K	481.13	Joback Method
cpg	243.77	J/mol×K	511.86	Joback Method
cpg	252.68	J/mol×K	542.58	Joback Method
cpg	261.25	J/mol×K	573.31	Joback Method
cpg	269.47	J/mol×K	604.04	Joback Method
cpg	277.34	J/mol×K	634.77	Joback Method
dvisc	0.0030315	Pa×s	259.46	Joback Method
dvisc	0.0016707	Pa×s	291.28	Joback Method
dvisc	0.0010354	Pa×s	323.11	Joback Method
dvisc	0.0006992	Pa×s	354.93	Joback Method
dvisc	0.0005036	Pa×s	386.75	Joback Method
dvisc	0.0003813	Pa×s	418.58	Joback Method
dvisc	0.0003003	Pa×s	450.40	Joback Method

Sources

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=C77877942&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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