Chloromethyl heptanoate

Other names: Heptanoic acid, chloromethyl ester
Inchi: InChI=1S/C8H15ClO2/c1-2-3-4-5-6-8(10)11-7-9/h2-7H2,1H3
InchiKey: JUBQFNSRJOLWED-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CCCCCCC(=O)OCCl
Mol. weight [g/mol]: 178.66
CAS: 76068-79-6

Physical Properties

Property code	Value	Unit	Source
gf	-229.37	kJ/mol	Joback Method
hf	-468.99	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.696		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1181.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1197.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1565.00		NIST Webbook
tb	496.16	K	Joback Method
tc	677.00	K	Joback Method
tf	282.00	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	307.66	J/mol×K	496.16	Joback Method
cpg	362.34	J/mol×K	646.86	Joback Method
cpg	352.32	J/mol×K	616.72	Joback Method
cpg	341.84	J/mol×K	586.58	Joback Method
cpg	330.91	J/mol×K	556.44	Joback Method
cpg	319.52	J/mol×K	526.30	Joback Method
cpg	371.92	J/mol×K	677.00	Joback Method
dvisc	0.0002618	Pa×s	496.16	Joback Method
dvisc	0.0003363	Pa×s	460.47	Joback Method
dvisc	0.0004506	Pa×s	424.77	Joback Method
dvisc	0.0006370	Pa×s	389.08	Joback Method
dvisc	0.0009658	Pa×s	353.39	Joback Method
dvisc	0.0016080	Pa×s	317.69	Joback Method
dvisc	0.0030458	Pa×s	282.00	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76068796&Units=SI
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

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