Chloromethyl 7-chloro-octanoate

Other names: 7-Chlorooctanoic acid, chloromethyl ester
Inchi: InChI=1S/C9H16Cl2O2/c1-8(11)5-3-2-4-6-9(12)13-7-10/h8H,2-7H2,1H3
InchiKey: RVCBGSJHWXKROV-UHFFFAOYSA-N
Formula: C9H16Cl2O2
SMILES: CC(Cl)CCCCCC(=O)OCCl
Mol. weight [g/mol]: 227.13
CAS: 80418-69-5

Physical Properties

Property code	Value	Unit	Source
gf	-235.32	kJ/mol	Joback Method
hf	-510.65	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	53.17	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.304		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpol	1484.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1498.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2121.00		NIST Webbook
ripol	2086.00		NIST Webbook
tb	556.03	K	Joback Method
tc	743.61	K	Joback Method
tf	308.19	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.33	J/mol×K	556.03	Joback Method

cpg	392.87	J/mol×K	587.29	Joback Method
cpg	404.84	J/mol×K	618.56	Joback Method
cpg	416.25	J/mol×K	649.82	Joback Method
cpg	427.10	J/mol×K	681.08	Joback Method
cpg	437.41	J/mol×K	712.35	Joback Method
cpg	447.18	J/mol×K	743.61	Joback Method
dvisc	0.0034137	Pa×s	308.19	Joback Method
dvisc	0.0016431	Pa×s	349.50	Joback Method
dvisc	0.0009231	Pa×s	390.80	Joback Method
dvisc	0.0005790	Pa×s	432.11	Joback Method
dvisc	0.0003940	Pa×s	473.42	Joback Method
dvisc	0.0002852	Pa×s	514.72	Joback Method
dvisc	0.0002166	Pa×s	556.03	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418695&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