Chloromethyl 3-chloroheptanoate

Other names: 3-Chloroheptanoic acid, chloromethyl ester
Inchi: InChI=1S/C8H14Cl2O2/c1-2-3-4-7(10)5-8(11)12-6-9/h7H,2-6H2,1H3
InchiKey: HJUPGERNLBGVLC-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: CCCCC(Cl)CC(=O)OCCl
Mol. weight [g/mol]: 213.10
CAS: 80418-59-3

Physical Properties

Property code	Value	Unit	Source
gf	-243.74	kJ/mol	Joback Method
hf	-490.01	kJ/mol	Joback Method
hfus	24.13	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.914		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1313.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1328.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1348.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1854.00		NIST Webbook
tb	533.15	K	Joback Method
tc	722.96	K	Joback Method
tf	296.92	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.71	J/mol×K	533.15	Joback Method
cpg	346.37	J/mol×K	564.79	Joback Method
cpg	357.50	J/mol×K	596.42	Joback Method
cpg	368.12	J/mol×K	628.06	Joback Method
cpg	378.23	J/mol×K	659.69	Joback Method
cpg	387.84	J/mol×K	691.33	Joback Method
cpg	396.95	J/mol×K	722.96	Joback Method
dvisc	0.0035993	Pa×s	296.92	Joback Method
dvisc	0.0017614	Pa×s	336.29	Joback Method
dvisc	0.0010012	Pa×s	375.66	Joback Method
dvisc	0.0006335	Pa×s	415.03	Joback Method
dvisc	0.0004339	Pa×s	454.41	Joback Method
dvisc	0.0003157	Pa×s	493.78	Joback Method
dvisc	0.0002408	Pa×s	533.15	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=C80418593&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