Chloromethyl 8-chloro-octanoate

Other names: 8-Chlorooctanoic acid, chloromethyl ester
Inchi: InChI=1S/C9H16Cl2O2/c10-7-5-3-1-2-4-6-9(12)13-8-11/h1-8H2
InchiKey: YEDAJMGEJCGDOV-UHFFFAOYSA-N
Formula: C9H16Cl2O2
SMILES: O=C(CCCCCCCCl)OCCl
Mol. weight [g/mol]: 227.13
CAS: 80418-70-8

Physical Properties

Property code	Value	Unit	Source
gf	-232.88	kJ/mol	Joback Method
hf	-505.37	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.305		Crippen Method
mcvol	169.590	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1545.00		NIST Webbook
ripol	2191.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2206.00		NIST Webbook
tb	556.47	K	Joback Method
tc	740.45	K	Joback Method
tf	323.19	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.98	J/mol×K	556.47	Joback Method
cpg	392.22	J/mol×K	587.13	Joback Method

cpg	403.92	J/mol×K	617.80	Joback Method
cpg	415.09	J/mol×K	648.46	Joback Method
cpg	425.73	J/mol×K	679.13	Joback Method
cpg	435.85	J/mol×K	709.79	Joback Method
cpg	445.47	J/mol×K	740.45	Joback Method
dvisc	0.0026055	Pa×s	323.19	Joback Method
dvisc	0.0014003	Pa×s	362.07	Joback Method
dvisc	0.0008489	Pa×s	400.95	Joback Method
dvisc	0.0005623	Pa×s	439.83	Joback Method
dvisc	0.0003982	Pa×s	478.71	Joback Method
dvisc	0.0002970	Pa×s	517.59	Joback Method
dvisc	0.0002308	Pa×s	556.47	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=C80418708&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