Chloromethyl 5-chlorononanoate

Other names: 5-Chlorononanoic acid, chloromethyl ester
Inchi: InChI=1S/C10H18Cl2O2/c1-2-3-5-9(12)6-4-7-10(13)14-8-11/h9H,2-8H2,1H3
InchiKey: MJVJQTXCHDQYKX-UHFFFAOYSA-N
Formula: C10H18Cl2O2
SMILES: CCCCC(Cl)CCCC(=O)OCCl
Mol. weight [g/mol]: 241.16
CAS: 80418-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-226.90	kJ/mol	Joback Method
hf	-531.29	kJ/mol	Joback Method
hfus	29.31	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.694		Crippen Method
mcvol	183.680	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1562.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1561.00		NIST Webbook
ripol	2123.00		NIST Webbook
ripol	2149.00		NIST Webbook
ripol	2160.00		NIST Webbook
tb	578.91	K	Joback Method
tc	764.42	K	Joback Method
tf	319.46	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.73	J/mol×K	578.91	Joback Method

cpg	441.05	J/mol×K	609.83	Joback Method
cpg	453.75	J/mol×K	640.75	Joback Method
cpg	465.85	J/mol×K	671.67	Joback Method
cpg	477.36	J/mol×K	702.58	Joback Method
cpg	488.28	J/mol×K	733.50	Joback Method
cpg	498.63	J/mol×K	764.42	Joback Method
dvisc	0.0032066	Pa×s	319.46	Joback Method
dvisc	0.0015197	Pa×s	362.70	Joback Method
dvisc	0.0008444	Pa×s	405.94	Joback Method
dvisc	0.0005254	Pa×s	449.19	Joback Method
dvisc	0.0003553	Pa×s	492.43	Joback Method
dvisc	0.0002560	Pa×s	535.67	Joback Method
dvisc	0.0001937	Pa×s	578.91	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=C80418742&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