Chloromethyl 7-chloroheptanoate

Other names: 7-Chloroheptanoic acid, chloromethyl ester
Inchi: InChI=1S/C8H14Cl2O2/c9-6-4-2-1-3-5-8(11)12-7-10/h1-7H2
InchiKey: MWONBSQQAQAREF-UHFFFAOYSA-N
Formula: C8H14Cl2O2
SMILES: O=C(CCCCCCCl)OCCl
Mol. weight [g/mol]: 213.10
CAS: 80418-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-241.30	kJ/mol	Joback Method
hf	-484.73	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	51.33	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.915		Crippen Method
mcvol	155.500	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1443.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1452.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2105.00		NIST Webbook
tb	533.59	K	Joback Method
tc	719.60	K	Joback Method
tf	311.92	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.38	J/mol×K	533.59	Joback Method
cpg	345.75	J/mol×K	564.59	Joback Method
cpg	356.61	J/mol×K	595.59	Joback Method
cpg	366.99	J/mol×K	626.59	Joback Method
cpg	376.89	J/mol×K	657.60	Joback Method
cpg	386.31	J/mol×K	688.60	Joback Method
cpg	395.27	J/mol×K	719.60	Joback Method
dvisc	0.0027181	Pa×s	311.92	Joback Method
dvisc	0.0014880	Pa×s	348.87	Joback Method
dvisc	0.0009142	Pa×s	385.81	Joback Method
dvisc	0.0006116	Pa×s	422.75	Joback Method
dvisc	0.0004365	Pa×s	459.70	Joback Method
dvisc	0.0003275	Pa×s	496.64	Joback Method
dvisc	0.0002557	Pa×s	533.59	Joback Method

Sources

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=C80418639&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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