Chloromethyl decanoate

Other names: Decanoic acid, chloromethyl ester
Inchi: InChI=1S/C11H21ClO2/c1-2-3-4-5-6-7-8-9-11(13)14-10-12/h2-10H2,1H3
InchiKey: UXAJBSZQOZOHEI-UHFFFAOYSA-N
Formula: C11H21ClO2
SMILES: CCCCCCCCCC(=O)OCCl
Mol. weight [g/mol]: 220.74
CAS: 67317-62-8

Physical Properties

Property code	Value	Unit	Source
gf	-204.11	kJ/mol	Joback Method
hf	-530.91	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.867		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1479.00		NIST Webbook
rinpol	1470.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1895.00		NIST Webbook
ripol	1872.00		NIST Webbook
tb	564.80	K	Joback Method
tc	740.70	K	Joback Method
tf	315.81	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.60	J/mol×K	564.80	Joback Method
cpg	512.59	J/mol×K	711.39	Joback Method
cpg	500.56	J/mol×K	682.07	Joback Method
cpg	487.95	J/mol×K	652.75	Joback Method
cpg	474.76	J/mol×K	623.43	Joback Method
cpg	460.98	J/mol×K	594.12	Joback Method
cpg	524.06	J/mol×K	740.70	Joback Method
dvisc	0.0001982	Pa×s	564.80	Joback Method
dvisc	0.0002583	Pa×s	523.30	Joback Method
dvisc	0.0003523	Pa×s	481.80	Joback Method
dvisc	0.0005095	Pa×s	440.30	Joback Method
dvisc	0.0007956	Pa×s	398.81	Joback Method
dvisc	0.0013779	Pa×s	357.31	Joback Method
dvisc	0.0027568	Pa×s	315.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67317628&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

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