Chloromethyl 10-chlorodecanoate

Other names: 10-Chlorodecanoic acid, chloromethyl ester
Inchi: InChI=1S/C11H20Cl2O2/c12-9-7-5-3-1-2-4-6-8-11(14)15-10-13/h1-10H2
InchiKey: ZOBAMFUTBJXGTK-UHFFFAOYSA-N
Formula: C11H20Cl2O2
SMILES: O=C(CCCCCCCCCCl)OCCl
Mol. weight [g/mol]: 255.18
CAS: 80418-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-216.04	kJ/mol	Joback Method
hf	-546.65	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.086		Crippen Method
mcvol	197.770	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1747.00		NIST Webbook
rinpol	1761.00		NIST Webbook
ripol	2401.00		NIST Webbook
ripol	2349.00		NIST Webbook
ripol	2403.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2349.00		NIST Webbook
tb	602.23	K	Joback Method
tc	782.71	K	Joback Method
tf	345.73	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.39	J/mol×K	602.23	Joback Method
cpg	490.11	J/mol×K	632.31	Joback Method
cpg	503.20	J/mol×K	662.39	Joback Method
cpg	515.68	J/mol×K	692.47	Joback Method
cpg	527.56	J/mol×K	722.55	Joback Method
cpg	538.85	J/mol×K	752.63	Joback Method
cpg	549.56	J/mol×K	782.71	Joback Method
dvisc	0.0023252	Pa×s	345.73	Joback Method
dvisc	0.0012081	Pa×s	388.48	Joback Method
dvisc	0.0007147	Pa×s	431.23	Joback Method
dvisc	0.0004648	Pa×s	473.98	Joback Method
dvisc	0.0003246	Pa×s	516.73	Joback Method
dvisc	0.0002394	Pa×s	559.48	Joback Method
dvisc	0.0001844	Pa×s	602.23	Joback Method

Sources

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=C80418877&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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