3-Chloroundecanoic acid, methyl ester

Inchi: InChI=1S/C12H23ClO2/c1-3-4-5-6-7-8-9-11(13)10-12(14)15-2/h11H,3-10H2,1-2H3
InchiKey: IXIZFSLPLYLYDO-UHFFFAOYSA-N
Formula: C12H23ClO2
SMILES: CCCCCCCCC(Cl)CC(=O)OC
Mol. weight [g/mol]: 234.76

Physical Properties

Property code	Value	Unit	Source
gf	-198.13	kJ/mol	Joback Method
hf	-556.83	kJ/mol	Joback Method
hfus	30.30	kJ/mol	Joback Method
hvap	55.46	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.907		Crippen Method
mcvol	199.620	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1555.00		NIST Webbook
ripol	1949.00		NIST Webbook
ripol	1949.00		NIST Webbook
tb	587.24	K	Joback Method
tc	764.85	K	Joback Method
tf	312.08	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.78	J/mol×K	587.24	Joback Method
cpg	566.97	J/mol×K	735.25	Joback Method
cpg	554.22	J/mol×K	705.64	Joback Method
cpg	540.84	J/mol×K	676.04	Joback Method
cpg	526.82	J/mol×K	646.44	Joback Method
cpg	512.13	J/mol×K	616.84	Joback Method
cpg	579.10	J/mol×K	764.85	Joback Method

dvisc	0.0001665	Pa×s	587.24	Joback Method
dvisc	0.0002228	Pa×s	541.38	Joback Method
dvisc	0.0003146	Pa×s	495.52	Joback Method
dvisc	0.0004765	Pa×s	449.66	Joback Method
dvisc	0.0007932	Pa×s	403.80	Joback Method
dvisc	0.0015046	Pa×s	357.94	Joback Method
dvisc	0.0034450	Pa×s	312.08	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=R309338&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

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