12-Chlorododecanoic acid, chloromethyl ester

Inchi: InChI=1S/C13H24Cl2O2/c14-11-9-7-5-3-1-2-4-6-8-10-13(16)17-12-15/h1-12H2
InchiKey: RHQDLXULLWJVQL-UHFFFAOYSA-N
Formula: C13H24Cl2O2
SMILES: O=C(CCCCCCCCCCCCl)OCCl
Mol. weight [g/mol]: 283.23

Physical Properties

Property code	Value	Unit	Source
gf	-199.20	kJ/mol	Joback Method
hf	-587.93	kJ/mol	Joback Method
hfus	40.61	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.866		Crippen Method
mcvol	225.950	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	1960.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1958.00		NIST Webbook
ripol	2601.00		NIST Webbook
ripol	2597.00		NIST Webbook
ripol	2567.00		NIST Webbook
tb	647.99	K	Joback Method
tc	826.05	K	Joback Method
tf	368.27	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.10	J/mol×K	647.99	Joback Method
cpg	594.00	J/mol×K	677.67	Joback Method
cpg	608.19	J/mol×K	707.34	Joback Method

cpg	621.71	J/mol×K	737.02	Joback Method
cpg	634.55	J/mol×K	766.70	Joback Method
cpg	646.75	J/mol×K	796.37	Joback Method
cpg	658.31	J/mol×K	826.05	Joback Method
dvisc	0.0020083	Pa×s	368.27	Joback Method
dvisc	0.0010123	Pa×s	414.89	Joback Method
dvisc	0.0005859	Pa×s	461.51	Joback Method
dvisc	0.0003750	Pa×s	508.13	Joback Method
dvisc	0.0002586	Pa×s	554.75	Joback Method
dvisc	0.0001890	Pa×s	601.37	Joback Method
dvisc	0.0001445	Pa×s	647.99	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=R249484&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