2-Chlorododecanoic acid, chloromethyl ester

Inchi: InChI=1S/C13H24Cl2O2/c1-2-3-4-5-6-7-8-9-10-12(15)13(16)17-11-14/h12H,2-11H2,1H3
InchiKey: SBSPUQUQGPCHIO-UHFFFAOYSA-N
Formula: C13H24Cl2O2
SMILES: CCCCCCCCCCC(Cl)C(=O)OCCl
Mol. weight [g/mol]: 283.23
CAS: 80418-98-0

Physical Properties

Property code	Value	Unit	Source
gf	-201.64	kJ/mol	Joback Method
hf	-593.21	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.864		Crippen Method
mcvol	225.950	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1840.00		NIST Webbook
ripol	2320.00		NIST Webbook
ripol	2315.00		NIST Webbook
ripol	2305.00		NIST Webbook
ripol	2305.00		NIST Webbook
tb	647.55	K	Joback Method
tc	828.32	K	Joback Method
tf	353.27	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	579.55	J/mol×K	647.55	Joback Method
cpg	594.71	J/mol×K	677.68	Joback Method
cpg	609.14	J/mol×K	707.81	Joback Method
cpg	622.86	J/mol×K	737.94	Joback Method
cpg	635.88	J/mol×K	768.06	Joback Method
cpg	648.22	J/mol×K	798.19	Joback Method
cpg	659.91	J/mol×K	828.32	Joback Method
dvisc	0.0025326	Pa×s	353.27	Joback Method
dvisc	0.0011518	Pa×s	402.32	Joback Method
dvisc	0.0006217	Pa×s	451.36	Joback Method
dvisc	0.0003786	Pa×s	500.41	Joback Method
dvisc	0.0002520	Pa×s	549.46	Joback Method
dvisc	0.0001792	Pa×s	598.50	Joback Method
dvisc	0.0001343	Pa×s	647.55	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C80418980&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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