

5-Chlorododecanoic acid, chloromethyl ester

Other names:	Chloromethyl 5-chlorododecanoate #
Inchi:	InChI=1S/C13H24Cl2O2/c1-2-3-4-5-6-8-12(15)9-7-10-13(16)17-11-14/h12H,2-11H2,1H3
InchiKey:	NHSXKNLOSXLLRZ-UHFFFAOYSA-N
Formula:	C13H24Cl2O2
SMILES:	CCCCCCCC(Cl)CCCC(=O)OCCI
Mol. weight [g/mol]:	283.23
CAS:	80419-01-8

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
ripol	1858.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1897.00		NIST Webbook
ripol	1872.00		NIST Webbook
ripol	2432.00		NIST Webbook
ripol	2432.00		NIST Webbook
ripol	2457.00		NIST Webbook
ripol	2452.00		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	Paxs	353.27	Joback Method
dvisc	0.0011518	Paxs	402.32	Joback Method
dvisc	0.0006217	Paxs	451.36	Joback Method
dvisc	0.0003786	Paxs	500.41	Joback Method
dvisc	0.0002520	Paxs	549.46	Joback Method
dvisc	0.0001792	Paxs	598.50	Joback Method
dvisc	0.0001343	Paxs	647.55	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=C80419018&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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