

Chloromethyl 4-chlorododecanoate

Other names:	4-Chlorododecanoic acid, chloromethyl ester
Inchi:	InChI=1S/C13H24Cl2O2/c1-2-3-4-5-6-7-8-12(15)9-10-13(16)17-11-14/h12H,2-11H2,1H3
InchiKey:	ZXYVRYZSZYAFKI-UHFFFAOYSA-N
Formula:	C13H24Cl2O2
SMILES:	CCCCCCCCC(Cl)CCC(=O)OCCI
Mol. weight [g/mol]:	283.23
CAS:	80419-00-7

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	1863.00		NIST Webbook
rinpol	1859.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1850.00		NIST Webbook
ripol	2424.00		NIST Webbook
ripol	2444.00		NIST Webbook
ripol	2448.00		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/molxK	647.55	Joback Method

cpg	594.71	J/molxK	677.68	Joback Method
cpg	609.14	J/molxK	707.81	Joback Method
cpg	622.86	J/molxK	737.94	Joback Method
cpg	635.88	J/molxK	768.06	Joback Method
cpg	648.22	J/molxK	798.19	Joback Method
cpg	659.91	J/molxK	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

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=C80419007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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