

3-Chloroundecanoic acid, chloromethyl ester

Inchi: InChI=1S/C12H22Cl2O2/c1-2-3-4-5-6-7-8-11(14)9-12(15)16-10-13/h11H,2-10H2,1H3
InchiKey: CFGPHVBCOWJONO-UHFFFAOYSA-N
Formula: C12H22Cl2O2
SMILES: CCCCCCCC(Cl)CC(=O)OCCI
Mol. weight [g/mol]: 269.21

Physical Properties

Property code	Value	Unit	Source
gf	-210.06	kJ/mol	Joback Method
hf	-572.57	kJ/mol	Joback Method
hfus	34.49	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.474		Crippen Method
mcvol	211.860	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
ripol	1730.00		NIST Webbook
ripol	1746.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2273.00		NIST Webbook
ripol	2273.00		NIST Webbook
tb	624.67	K	Joback Method
tc	806.72	K	Joback Method
tf	342.00	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.44	J/molxK	624.67	Joback Method

cpg	593.73	J/molxK	776.38	Joback Method
cpg	581.80	J/molxK	746.04	Joback Method
cpg	569.22	J/molxK	715.70	Joback Method
cpg	555.97	J/molxK	685.35	Joback Method
cpg	542.05	J/molxK	655.01	Joback Method
cpg	605.03	J/molxK	806.72	Joback Method
dvisc	0.0001524	Paxs	624.67	Joback Method
dvisc	0.0002028	Paxs	577.56	Joback Method
dvisc	0.0002840	Paxs	530.45	Joback Method
dvisc	0.0004246	Paxs	483.33	Joback Method
dvisc	0.0006925	Paxs	436.22	Joback Method
dvisc	0.0012714	Paxs	389.11	Joback Method
dvisc	0.0027597	Paxs	342.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249508&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

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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