

3-Chloropropionic acid, undec-2-enyl ester

Inchi:	InChI=1S/C14H25ClO2/c1-2-3-4-5-6-7-8-9-10-13-17-14(16)11-12-15/h9-10H,2-8,11-13H
InchiKey:	SRHPHYGOUXFJTB-MDZDMXLPSA-N
Formula:	C14H25ClO2
SMILES:	CCCCCCCCC=CCOC(=O)CCCl
Mol. weight [g/mol]:	260.80

Physical Properties

Property code	Value	Unit	Source
gf	-98.63	kJ/mol	Joback Method
hf	-475.61	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.465		Crippen Method
mcvol	223.500	ml/mol	McGowan Method
pc	1598.72	kPa	Joback Method
rinqol	1795.00		NIST Webbook
tb	637.60	K	Joback Method
tc	816.02	K	Joback Method
tf	344.54	K	Joback Method
vc	0.873	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.89	J/molxK	637.60	Joback Method
cpg	595.62	J/molxK	667.34	Joback Method
cpg	610.61	J/molxK	697.07	Joback Method
cpg	624.89	J/molxK	726.81	Joback Method
cpg	638.48	J/molxK	756.55	Joback Method
cpg	651.41	J/molxK	786.29	Joback Method
cpg	663.69	J/molxK	816.02	Joback Method
dvisc	0.0021188	Paxs	344.54	Joback Method
dvisc	0.0009782	Paxs	393.38	Joback Method

dvisc	0.0005357	Paxs	442.23	Joback Method
dvisc	0.0003307	Paxs	491.07	Joback Method
dvisc	0.0002228	Paxs	539.91	Joback Method
dvisc	0.0001603	Paxs	588.76	Joback Method
dvisc	0.0001212	Paxs	637.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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