

Undecanoic acid, 11-chloro-

Inchi:	InChI=1S/C11H21ClO2/c12-10-8-6-4-2-1-3-5-7-9-11(13)14/h1-10H2,(H,13,14)
InchiKey:	GVZXFVFTBUYBJD-UHFFFAOYSA-N
Formula:	C11H21ClO2
SMILES:	O=C(O)CCCCCCCCCCI
Mol. weight [g/mol]:	220.74
CAS:	1860-44-2

Physical Properties

Property code	Value	Unit	Source
gf	-235.93	kJ/mol	Joback Method
hf	-550.92	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	67.89	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.821		Crippen Method
mvol	185.530	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1778.00		NIST Webbook
tb	634.56	K	Joback Method
tc	805.69	K	Joback Method
tf	354.40	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.86	J/molxK	634.56	Joback Method
cpg	493.35	J/molxK	663.08	Joback Method
cpg	505.27	J/molxK	691.60	Joback Method
cpg	516.64	J/molxK	720.12	Joback Method
cpg	527.48	J/molxK	748.65	Joback Method
cpg	537.80	J/molxK	777.17	Joback Method
cpg	547.63	J/molxK	805.69	Joback Method
dvisc	0.0055871	Paxs	354.40	Joback Method

dvisc	0.0017794	Paxs	401.09	Joback Method
dvisc	0.0007194	Paxs	447.79	Joback Method
dvisc	0.0003451	Paxs	494.48	Joback Method
dvisc	0.0001879	Paxs	541.17	Joback Method
dvisc	0.0001127	Paxs	587.87	Joback Method
dvisc	0.0000729	Paxs	634.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1860442&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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