

3-Chloropropionic acid, nonyl ester

Other names:	Propanoic acid, 3-chloro, nonyl ester Nonyl 3-chloropropanoate
Inchi:	InChI=1S/C12H23ClO2/c1-2-3-4-5-6-7-8-11-15-12(14)9-10-13/h2-11H2,1H3
InchiKey:	TVEXZMIDIHNANR-UHFFFAOYSA-N
Formula:	C12H23ClO2
SMILES:	CCCCCCCCCOC(=O)CCCl
Mol. weight [g/mol]:	234.76
CAS:	74306-05-1

Physical Properties

Property code	Value	Unit	Source
gf	-195.69	kJ/mol	Joback Method
hf	-551.55	kJ/mol	Joback Method
hfus	33.82	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.909		Crippen Method
mvol	199.620	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
ripol	1595.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1603.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1604.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2084.00		NIST Webbook
tb	587.68	K	Joback Method
tc	762.26	K	Joback Method
tf	327.08	K	Joback Method
vc	0.780	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.42	J/molxK	587.68	Joback Method
cpg	511.47	J/molxK	616.78	Joback Method
cpg	525.87	J/molxK	645.87	Joback Method
cpg	539.64	J/molxK	674.97	Joback Method
cpg	552.80	J/molxK	704.07	Joback Method
cpg	565.36	J/molxK	733.17	Joback Method
cpg	577.32	J/molxK	762.26	Joback Method
dvisc	0.0026085	Paxs	327.08	Joback Method
dvisc	0.0012830	Paxs	370.51	Joback Method
dvisc	0.0007323	Paxs	413.95	Joback Method
dvisc	0.0004650	Paxs	457.38	Joback Method
dvisc	0.0003194	Paxs	500.81	Joback Method
dvisc	0.0002330	Paxs	544.25	Joback Method
dvisc	0.0001781	Paxs	587.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74306051&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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