

Dodecanoyl chloride

Other names:	Lauroyl chloride n-Dodecanoyl chloride Lauric acid, chloride Dodecanoic acid, chloride
Inchi:	InChI=1S/C12H23ClO/c1-2-3-4-5-6-7-8-9-10-11-12(13)14/h2-11H2,1H3
InchiKey:	NQGIJDNPuzeBRU-UHFFFAOYSA-N
Formula:	C12H23ClO
SMILES:	CCCCCCCCCCCC(=O)Cl
Mol. weight [g/mol]:	218.76
CAS:	112-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-90.69	kJ/mol	Joback Method
hf	-419.33	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	53.44	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.673		Crippen Method
mcvol	193.750	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
tb	565.26	K	Joback Method
tc	740.36	K	Joback Method
tf	304.85	K	Joback Method
vc	0.762	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.04	J/mol×K	565.26	Joback Method
cpg	484.33	J/mol×K	594.44	Joback Method
cpg	498.95	J/mol×K	623.63	Joback Method
cpg	512.91	J/mol×K	652.81	Joback Method
cpg	526.23	J/mol×K	681.99	Joback Method

cpg	538.94	J/molxK	711.18	Joback Method
cpg	551.06	J/molxK	740.36	Joback Method
dvisc	0.0037253	Paxs	304.85	Joback Method
dvisc	0.0017430	Paxs	348.25	Joback Method
dvisc	0.0009651	Paxs	391.65	Joback Method
dvisc	0.0006012	Paxs	435.06	Joback Method
dvisc	0.0004081	Paxs	478.46	Joback Method
dvisc	0.0002955	Paxs	521.86	Joback Method
dvisc	0.0002248	Paxs	565.26	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	1.50	NIST Webbook
tbrp	418.20	K	2.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112163&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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