

Stearic acid chloride

Other names:	Stearoyl chloride Octadecanoyl-chloride-
Inchi:	InChI=1S/C18H35ClO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-17H2,1
InchiKey:	WTBAHSZERDXKKZ-UHFFFAOYSA-N
Formula:	C18H35ClO
SMILES:	CCCCCCCCCCCCCCCC(=O)Cl
Mol. weight [g/mol]:	302.92
CAS:	112-76-5

Physical Properties

Property code	Value	Unit	Source
gf	-40.17	kJ/mol	Joback Method
hf	-543.17	kJ/mol	Joback Method
hfus	48.17	kJ/mol	Joback Method
h vap	66.79	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.013		Crippen Method
m cvol	278.290	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
tb	702.54	K	Joback Method
tc	874.89	K	Joback Method
tf	372.47	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.90	J/mol×K	702.54	Joback Method
cpg	812.09	J/mol×K	731.27	Joback Method
cpg	829.44	J/mol×K	759.99	Joback Method
cpg	845.97	J/mol×K	788.72	Joback Method
cpg	861.71	J/mol×K	817.44	Joback Method
cpg	876.70	J/mol×K	846.17	Joback Method
cpg	890.95	J/mol×K	874.89	Joback Method

dvisc	0.0023561	Paxs	372.47	Joback Method
dvisc	0.0010201	Paxs	427.48	Joback Method
dvisc	0.0005346	Paxs	482.49	Joback Method
dvisc	0.0003198	Paxs	537.50	Joback Method
dvisc	0.0002104	Paxs	592.52	Joback Method
dvisc	0.0001487	Paxs	647.53	Joback Method
dvisc	0.0001109	Paxs	702.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	449.20	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112765&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
mccvol:	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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