

Palmitoyl chloride

Other names:	Hexadecanoyl-chloride- Palmitic acid chloride
Inchi:	InChI=1S/C16H31ClO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3
InchiKey:	ARBOVOVUTSQWSS-UHFFFAOYSA-N
Formula:	C16H31ClO
SMILES:	CCCCCCCCCCCCCCCC(=O)Cl
Mol. weight [g/mol]:	274.87
CAS:	112-67-4

Physical Properties

Property code	Value	Unit	Source
gf	-57.01	kJ/mol	Joback Method
hf	-501.89	kJ/mol	Joback Method
hfus	42.99	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	6.233		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
tb	656.78	K	Joback Method
tc	828.55	K	Joback Method
tf	349.93	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.32	J/mol×K	656.78	Joback Method
cpg	697.67	J/mol×K	685.41	Joback Method
cpg	714.24	J/mol×K	714.04	Joback Method
cpg	730.04	J/mol×K	742.66	Joback Method
cpg	745.11	J/mol×K	771.29	Joback Method
cpg	759.47	J/mol×K	799.92	Joback Method
cpg	773.14	J/mol×K	828.55	Joback Method

dvisc	0.0028254	Pa×s	349.93	Joback Method
dvisc	0.0012516	Pa×s	401.07	Joback Method
dvisc	0.0006665	Pa×s	452.21	Joback Method
dvisc	0.0004035	Pa×s	503.36	Joback Method
dvisc	0.0002679	Pa×s	554.50	Joback Method
dvisc	0.0001906	Pa×s	605.64	Joback Method
dvisc	0.0001430	Pa×s	656.78	Joback Method

Sources

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=C112674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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