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]: 274.88

Physical Properties

Property code	Value	Unit	Source
af	0.8170		Cheméo Relay (1.0)
gf	-57.01	kJ/mol	Joback Method
hf	-546.11	kJ/mol	Cheméo Relay (1.0)
hfus	42.99	kJ/mol	Joback Method
hvap	85.89	kJ/mol	Cheméo Relay (1.0)
ie	9.96	eV	Cheméo Relay (1.0)
log10ws	-6.95		Cheméo Relay (1.0)
logp	6.233		Crippen Method
mcvol	250.110	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
tb	567.85	K	Cheméo Relay (1.0)
tc	754.70	K	Cheméo Relay (1.0)
tf	307.94	K	Cheméo Relay (1.0)
vc	0.968	m3/kmol	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112674&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
ie: Ionization energy
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