

Palmitoleic acid

Other names:

(Z)-9-Hexadecenoic acid
(Z)-Palmitoleic acid
(Z)-hexadec-9-enoic acid
9-Hexadecenoic acid, (Z)-
9-cis-Hexadecenoic acid
Palmitolinoleic acid
cis-9-Hexadecenoic acid
cis-Hexadec-9-enoic acid
cis-Palmitoleic acid
cis-«delta»9-Hexadecenoic acid
cis-Â«deltaÂ»9-Hexadecenoic acid

Inchi:

InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h7-8H,2-6,9-15H2

InchiKey:

SECPZKHBENQXJG-FPLPWBNLSA-N

Formula:

C16H30O2

SMILES:

CCCCCCC=CCCCCCCC(=O)O

Mol. weight [g/mol]:

254.41

CAS:

373-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-101.68	kJ/mol	Joback Method
hf	-521.16	kJ/mol	Joback Method
hfl	-713.40	kJ/mol	NIST Webbook
hfus	43.09	kJ/mol	Joback Method
hvap	74.59	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.328		Crippen Method
mvol	239.440	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1939.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1933.00		NIST Webbook
rinpol	1929.00		NIST Webbook
rinpol	1931.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1931.00		NIST Webbook

rinpol	1942.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1957.10		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
rinpol	1952.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1958.00		NIST Webbook
ripol	2908.00		NIST Webbook
ripol	2904.00		NIST Webbook
ripol	2908.00		NIST Webbook
ripol	2960.00		NIST Webbook
ripol	2944.00		NIST Webbook
tb	715.69	K	Joback Method
tc	887.89	K	Joback Method
tf	375.75	K	Joback Method
vc	0.936	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.14	J/molxK	859.19	Joback Method
cpg	779.32	J/molxK	887.89	Joback Method
cpg	696.79	J/molxK	715.69	Joback Method
cpg	712.23	J/molxK	744.39	Joback Method
cpg	726.95	J/molxK	773.09	Joback Method
cpg	740.99	J/molxK	801.79	Joback Method
cpg	754.38	J/molxK	830.49	Joback Method
dvisc	0.0000302	Paxs	715.69	Joback Method
dvisc	0.0000474	Paxs	659.03	Joback Method
dvisc	0.0034930	Paxs	375.75	Joback Method
dvisc	0.0009417	Paxs	432.41	Joback Method

dvisc	0.0003440	Paxs	489.06	Joback Method
dvisc	0.0001549	Paxs	545.72	Joback Method
dvisc	0.0000810	Paxs	602.38	Joback Method
hfust	32.10	kJ/mol	275.20	NIST Webbook
hvapt	123.00	kJ/mol	298.15	Vaporization, Sublimation and Fusion Enthalpies of Some Saturated and Unsaturated Long Chain Fatty Acids by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.20	K	0.08	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46024e+01
Coeff. B	-5.30092e+03
Coeff. C	-1.16610e+02
Temperature range (K), min.	486.92
Temperature range (K), max.	687.16

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C373499&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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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