Heptadecanoic acid, methyl ester

Other names:	27:0, Me ester
	Margaric acid methyl ester
	Methyl heptadecanoate
	Methyl margarate
	methyl heptadecanoate (17:0)
	n-Heptadecanoic acid methyl ester
Inchi:	InChI=1S/C18H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20-2/h3-17H2,1-2
InchiKey:	HUEBIMLTDXKIPR-UHFFFAOYSA-N
Formula:	C18H36O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	284.48
CAS:	1731-92-6

Physical Properties

Property code	Value	Unit	Source
gf	-133.24	kJ/mol	Joback Method
hf	-659.65	kJ/mol	Joback Method
hfus	63.90	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	100.80 ± 1.00	kJ/mol	NIST Webbook
hvap	97.00 ± 1.20	kJ/mol	NIST Webbook
log10ws	-6.22		Crippen Method
logp	6.031		Crippen Method
mcvol	271.920	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2003.10		NIST Webbook
rinpol	2004.20		NIST Webbook
rinpol	2005.50		NIST Webbook
rinpol	2006.70		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	2009.30		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2014.00		NIST Webbook

rinpol	2011.00	NIST Webbook
rinpol	2007.00	NIST Webbook
rinpol	2013.00	NIST Webbook
rinpol	2013.00	NIST Webbook
rinpol	2009.00	NIST Webbook
rinpol	2028.00	NIST Webbook
rinpol	2008.00	NIST Webbook
rinpol	2008.00	NIST Webbook
rinpol	2010.00	NIST Webbook
rinpol	2028.00	NIST Webbook
rinpol	2030.00	NIST Webbook
rinpol	2009.00	NIST Webbook
rinpol	2009.00	NIST Webbook
rinpol	2021.00	NIST Webbook
rinpol	2008.00	NIST Webbook
rinpol	2024.00	NIST Webbook
rinpol	2026.00	NIST Webbook
rinpol	2001.90	NIST Webbook
rinpol	2022.00	NIST Webbook
rinpol	2037.00	NIST Webbook
rinpol	2007.00	NIST Webbook
rinpol	2005.00	NIST Webbook
rinpol	2029.00	NIST Webbook
rinpol	2007.00	NIST Webbook
rinpol	2006.00	NIST Webbook
rinpol	2028.00	NIST Webbook
rinpol	347.00	NIST Webbook
rinpol	347.10	NIST Webbook
rinpol	336.55	NIST Webbook
rinpol	336.74	NIST Webbook
rinpol	336.74	NIST Webbook
rinpol	336.74	NIST Webbook
rinpol	2030.00	NIST Webbook
rinpol	347.00	NIST Webbook
rinpol	2009.00	NIST Webbook
rinpol	2006.00	NIST Webbook
rinpol	2008.00	NIST Webbook
rinpol	2007.00	NIST Webbook
rinpol	2001.90	NIST Webbook
ripol	2295.00	NIST Webbook
ripol	2307.00	NIST Webbook
ripol	2307.00	NIST Webbook
ripol	2344.00	NIST Webbook
ripol	2309.00	NIST Webbook

ripol	2297.00		NIST Webbook
ripol	2309.00		NIST Webbook
ripol	2325.00		NIST Webbook
ripol	2329.00		NIST Webbook
tb	687.53	K	Joback Method
tc	855.83	K	Joback Method
tf	302.25 ± 0.40	K	NIST Webbook
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.54	J/mol×K	855.83	Joback Method
cpg	826.65	J/mol×K	743.63	Joback Method
cpg	843.80	J/mol×K	771.68	Joback Method
cpg	860.14	J/mol×K	799.73	Joback Method
cpg	808.70	J/mol×K	715.58	Joback Method
cpg	875.72	J/mol×K	827.78	Joback Method
cpg	789.92	J/mol×K	687.53	Joback Method
dvisc	0.0000953	Pa×s	687.53	Joback Method
dvisc	0.0001809	Pa×s	579.95	Joback Method
dvisc	0.0002749	Pa×s	526.15	Joback Method
dvisc	0.0008765	Pa×s	418.57	Joback Method
dvisc	0.0001278	Pa×s	633.74	Joback Method
dvisc	0.0004595	Pa×s	472.36	Joback Method
dvisc	0.0020226	Pa×s	364.78	Joback Method
hfust	48.10	kJ/mol	304.20	NIST Webbook
hvapt	84.40	kJ/mol	473.00	NIST Webbook
hvapt	89.00 ± 0.70	kJ/mol	353.00	NIST Webbook
hvapt	89.30	kJ/mol	350.00	NIST Webbook
hvapt	100.80	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography

pvap	0.05	kPa	408.15	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.03	kPa	399.20	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.04	kPa	402.35	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.04	kPa	405.30	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.06	kPa	412.20	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.02	kPa	391.30	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	2.72e-03	kPa	365.25	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

pvap	6.85e-04	kPa	347.95	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	2.98e-04	kPa	339.75	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	3.01e-03	kPa	366.85	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	3.95e-04	kPa	342.85	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	2.59e-04	kPa	337.90	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	3.71e-04	kPa	341.80	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	5.32e-04	kPa	345.85	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

pvap	8.03e-04	kPa	350.00	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.02	kPa	396.20	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.02	kPa	389.25	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.01	kPa	387.00	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	8.90e-03	kPa	382.25	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	5.80e-03	kPa	376.20	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	4.64e-03	kPa	372.30	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

pvap	3.77e-03	kPa	369.00	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	1.44e-03	kPa	357.50	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	1.95e-03	kPa	360.60	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.01	kPa	385.65	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	1.14e-03	kPa	354.30	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	7.72e-03	kPa	379.20	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	2.06e-03	kPa	362.50	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

pvap	0.02	kPa	393.40	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.74700e+01
Coeff. B	-6.23670e+03
Coeff. C	-1.14830e+02
Temperature range (K), min.	477.80
Temperature range (K), max.	627.78

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyl Octanoate to Methyl Hexadecanoate between 5 K and 390 K:	https://www.doi.org/10.1021/je0499364
Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics:	https://www.doi.org/10.1016/j.jct.2019.01.007
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731926&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
the vaporization enthaplies and vapor pressures of a series of unstaurated fattyacid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume