Pentadecanoic acid, methyl ester

Other names:	25:0, Me ester
	Methyl n-pentadecanoate
	Methyl pentadecanoate
	n-Pentadecanoic acid methyl ester
	pentadecanoic acid methyl ester
Inchi:	InChI=1S/C16H32O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18-2/h3-15H2,1-2H3
InchiKey:	XIUXKAZJZFLLDQ-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	256.42
CAS:	7132-64-1

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	89.30 ± 0.80	kJ/mol	NIST Webbook
hvap	88.00 ± 1.00	kJ/mol	NIST Webbook
hvap	93.50 ± 1.00	kJ/mol	NIST Webbook
hvap	93.49 ± 0.94	kJ/mol	NIST Webbook
hvap	91.60 ± 0.90	kJ/mol	NIST Webbook
hvap	88.80	kJ/mol	NIST Webbook
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1806.00		NIST Webbook
rinpol	1824.50		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	305.23		NIST Webbook

rinpol	314.60		NIST Webbook
rinpol	1811.00		NIST Webbook
rinpol	1807.00		NIST Webbook
ripol	2107.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2099.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	342.24	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method
hvapt	90.70	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48072e+01
Coeff. B	-4.82665e+03
Coeff. C	-9.90960e+01
Temperature range (K), min.	431.52
Temperature range (K), max.	607.40

Sources

the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography:	https://www.doi.org/10.1016/j.tca.2007.02.008
Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K:	https://www.doi.org/10.1021/je0499364
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=C7132641&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/ci990307l
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
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