Docosanoic acid, methyl ester

Other names:	22:0, Me ester
	Behenic acid, methyl ester
	Kemester 9022
	Methyl behenate
	Methyl behenoate
	Methyl docosanoate
	n-Docosanoic acid methyl ester
Inchi:	InChI=1S/C23H46O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)2
InchiKey:	QSQLTHHMFHEFIY-UHFFFAOYSA-N
Formula:	C23H46O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	354.61
CAS:	929-77-1

Physical Properties

Property code	Value	Unit	Source
chs	-14565.00 ± 0.40	kJ/mol	NIST Webbook
gf	-91.14	kJ/mol	Joback Method
hf	-762.85	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	126.10 ± 2.50	kJ/mol	NIST Webbook
hvap	126.00 ± 0.30	kJ/mol	NIST Webbook
hvap	126.10	kJ/mol	NIST Webbook
log10ws	-8.31		Crippen Method
logp	7.981		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2494.70		NIST Webbook
rinpol	2495.90		NIST Webbook
rinpol	2497.10		NIST Webbook
rinpol	2498.30		NIST Webbook
rinpol	2513.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2515.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2531.00		NIST Webbook

rinpol	2502.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2493.60		NIST Webbook
rinpol	2510.00		NIST Webbook
rinpol	2531.00		NIST Webbook
rinpol	2492.50		NIST Webbook
rinpol	2527.50		NIST Webbook
rinpol	2528.80		NIST Webbook
rinpol	2512.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2530.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2538.00		NIST Webbook
rinpol	2531.00		NIST Webbook
rinpol	2504.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2514.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2509.00		NIST Webbook
rinpol	2524.00		NIST Webbook
rinpol	2491.40		NIST Webbook
rinpol	419.20		NIST Webbook
rinpol	420.50		NIST Webbook
rinpol	420.60		NIST Webbook
rinpol	404.49		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2527.50		NIST Webbook
tb	801.93	K	Joback Method
tc	982.34	K	Joback Method
tf	421.13	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.55	J/mol×K	922.21	Joback Method
cpg	1204.49	J/mol×K	982.34	Joback Method
cpg	1188.50	J/mol×K	952.27	Joback Method
cpg	1093.53	J/mol×K	801.93	Joback Method
cpg	1114.64	J/mol×K	832.00	Joback Method

cpg	1134.65	J/mol×K	862.07	Joback Method
cpg	1153.61	J/mol×K	892.14	Joback Method
dvisc	0.0027087	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0025020	Pa×s	368.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0023169	Pa×s	373.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0047493	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0042736	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0038657	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0035133	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0032066	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0029392	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
hfust	82.30	kJ/mol	327.20	NIST Webbook
hfust	83.50	kJ/mol	327.20	NIST Webbook
hfust	82.30	kJ/mol	325.00	NIST Webbook
hfust	29.20	kJ/mol	324.99	NIST Webbook
hvapt	98.20	kJ/mol	503.00	NIST Webbook
hvapt	81.00	kJ/mol	498.00	NIST Webbook
hvapt	127.50	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	2.53807e+01
Coeff. B	-1.04203e+04
Coeff. C	-1.59063e+02
Temperature range (K), min.	574.33
Temperature range (K), max.	678.28

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Phase behaviour of high molecular mass methyl esters in supercritical ethane:	https://www.doi.org/10.1016/j.fluid.2011.08.015
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
Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel:	https://www.doi.org/10.1021/je1012235
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C929771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume