Heneicosanoic acid, methyl ester

Other names:	21:0 Me ester
	Methyl heneicosanoate
	Methyl heneicosanoate (C-21)
	Methyl henicosanoate
	methyl henicosaneate
Inchi:	InChI=1S/C22H44O2/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:	AJRICDSAJQHDSD-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	340.58
CAS:	6064-90-0

Physical Properties

Property code	Value	Unit	Source
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2428.80		NIST Webbook
rinpol	404.80		NIST Webbook
rinpol	2409.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	391.75		NIST Webbook
rinpol	2428.80		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2414.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2410.00		NIST Webbook
ripol	2748.00		NIST Webbook
ripol	2716.00		NIST Webbook
tb	779.05	K	Joback Method

tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1139.78	J/mol×K	955.69	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1031.01	J/mol×K	779.05	Joback Method
cpg	1051.60	J/mol×K	808.49	Joback Method
cpg	1071.17	J/mol×K	837.93	Joback Method
cpg	1089.74	J/mol×K	867.37	Joback Method
dvisc	0.0000557	Pa×s	779.05	Joback Method
dvisc	0.0001080	Pa×s	655.99	Joback Method
dvisc	0.0000754	Pa×s	717.52	Joback Method
dvisc	0.0013386	Pa×s	409.86	Joback Method
dvisc	0.0005575	Pa×s	471.39	Joback Method
dvisc	0.0002843	Pa×s	532.92	Joback Method
dvisc	0.0001666	Pa×s	594.45	Joback Method
hfust	75.10	kJ/mol	321.20	NIST Webbook
hvapt	95.60	kJ/mol	494.00	NIST Webbook
hvapt	116.30	kJ/mol	298.00	A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	480.20	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.18421e+01
Coeff. B	-8.72175e+03
Coeff. C	-1.43123e+02
Temperature range (K), min.	547.76
Temperature range (K), max.	670.74

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A Comparison of Results by Correlation Gas Chromatography with Another Gas Chromatographic Retention Time Technique. The Effects of Retention Time Coincidence on Vaporization Enthalpy and Vapor Pressure:	https://www.doi.org/10.1021/acs.jced.5b00444
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=C6064900&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume