Undecanoic acid, methyl ester

Other names:	Methyl ester of undecanoic acid
	Methyl undecanoate
	Methyl undecylenate
	methyl n-undecanoate
	n-Undecanoic acid methyl ester
Inchi:	InChI=1S/C12H24O2/c1-3-4-5-6-7-8-9-10-11-12(13)14-2/h3-11H2,1-2H3
InchiKey:	XPQPWPZFBULGKT-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	200.32
CAS:	1731-86-8

Physical Properties

Property code	Value	Unit	Source
chl	-7486.50 ± 1.30	kJ/mol	NIST Webbook
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	71.40 ± 0.30	kJ/mol	NIST Webbook
hvap	70.60	kJ/mol	NIST Webbook
hvap	70.80 ± 0.40	kJ/mol	NIST Webbook
hvap	71.37 ± 0.30	kJ/mol	NIST Webbook
hvap	72.40	kJ/mol	NIST Webbook
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1430.00		NIST Webbook

rinpol	1427.00		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1422.50		NIST Webbook
rinpol	1421.50		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1411.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1414.00		NIST Webbook
ripol	1696.60		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1732.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1711.60		NIST Webbook
ripol	1706.60		NIST Webbook
ripol	1701.80		NIST Webbook
ripol	1686.70		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1705.70		NIST Webbook
ripol	1704.60		NIST Webbook
ripol	1665.00		NIST Webbook
ripol	1728.70		NIST Webbook
tb	344.15 ± 2.00	K	NIST Webbook
tc	720.05	K	Joback Method
tf	261.80 ± 0.05	K	NIST Webbook
tt	262.00	K	Heat capacities of potential organic phase change materials

vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/mol×K	550.25	Joback Method
cpg	479.84	J/mol×K	578.55	Joback Method
cpg	494.90	J/mol×K	606.85	Joback Method
cpg	509.36	J/mol×K	635.15	Joback Method
cpg	523.23	J/mol×K	663.45	Joback Method
cpg	536.51	J/mol×K	691.75	Joback Method
cpg	549.22	J/mol×K	720.05	Joback Method
cpl	411.40	J/mol×K	303.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	415.90	J/mol×K	313.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	420.90	J/mol×K	323.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	426.10	J/mol×K	333.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	431.40	J/mol×K	343.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	436.70	J/mol×K	353.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters

cpl	441.80	J/mol×K	363.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
cpl	446.50	J/mol×K	373.15	Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters
dvisc	0.0001878	Pa×s	550.25	Joback Method
dvisc	0.0014485	Pa×s	339.34	Joback Method
dvisc	0.0008035	Pa×s	381.52	Joback Method
dvisc	0.0005012	Pa×s	423.70	Joback Method
dvisc	0.0003406	Pa×s	465.89	Joback Method
dvisc	0.0002467	Pa×s	508.07	Joback Method
dvisc	0.0030867	Pa×s	297.16	Joback Method
hvapt	66.10	kJ/mol	350.00	NIST Webbook
hvapt	67.00 ± 0.10	kJ/mol	340.00	NIST Webbook
hvapt	60.90	kJ/mol	433.00	NIST Webbook
pvap	3.58e-03	kPa	305.25	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	4.50e-03	kPa	307.81	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	5.57e-03	kPa	310.15	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	6.96e-03	kPa	312.67	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics

pvap	8.55e-03	kPa	315.06	Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics
pvap	0.01	kPa	317.52	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	1.55084e+01
Coeff. B	-4.64990e+03
Coeff. C	-8.42230e+01
Temperature range (K), min.	389.72
Temperature range (K), max.	540.23

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat capacities and thermal diffusivities of some n-alkanoic acid methyl esters:	https://www.doi.org/10.1016/j.jct.2018.09.024
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Fatty acids methyl esters: Complementary measurements and comprehensive analysis of vaporization thermodynamics:	https://www.doi.org/10.1016/j.jct.2019.01.007
Heat capacities of potential organic phase change materials:	https://www.doi.org/10.1016/j.jct.2018.08.014
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
Acree-Jr Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1731868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
tt:	Triple Point Temperature
vc:	Critical Volume