10-Undecenoic acid, methyl ester

Other names:	10-Hendecenoic acid, methyl ester
	Methyl 10-undecenate
	Methyl 10-undecenoate
	Methyl ester of 10-undecenoic acid
	Methyl undec-10-enylate
	Methyl undecenate
	Methyl undecenoate
	NSC 1273
	Undecenoic acid, methyl ester
	Undecylenic acid, methyl ester
	methyl undec-10-enoate
Inchi:	InChI=1S/C12H22O2/c1-3-4-5-6-7-8-9-10-11-12(13)14-2/h3H,1,4-11H2,2H3
InchiKey:	KISVAASFGZJBCY-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	C=CCCCCCCCCC(=O)OC
Mol. weight [g/mol]:	198.30
CAS:	111-81-9

Physical Properties

Property code	Value	Unit	Source
gf	-95.92	kJ/mol	Joback Method
hf	-410.38	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.466		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	1396.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1395.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1417.30		NIST Webbook
ripol	1718.00		NIST Webbook

ripol	1733.00		NIST Webbook
ripol	1718.00		NIST Webbook
tb	521.20	K	NIST Webbook
tc	719.58	K	Joback Method
tf	295.40	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.24	J/mol×K	719.58	Joback Method
cpg	514.06	J/mol×K	690.81	Joback Method
cpg	501.31	J/mol×K	662.03	Joback Method
cpg	487.98	J/mol×K	633.26	Joback Method
cpg	474.05	J/mol×K	604.48	Joback Method
cpg	459.51	J/mol×K	575.71	Joback Method
cpg	444.34	J/mol×K	546.93	Joback Method
dvisc	0.0029144	Pa×s	295.40	Joback Method
dvisc	0.0001931	Pa×s	546.93	Joback Method
dvisc	0.0002516	Pa×s	505.01	Joback Method
dvisc	0.0003439	Pa×s	463.09	Joback Method
dvisc	0.0005002	Pa×s	421.17	Joback Method
dvisc	0.0007904	Pa×s	379.24	Joback Method
dvisc	0.0013996	Pa×s	337.32	Joback Method
hvapt	59.20	kJ/mol	460.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55377e+01
Coeff. B	-4.75178e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	397.62
Temperature range (K), max.	550.70

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	280.15	897.46
100.00	293.15	886.83
100.00	303.15	878.63
100.00	313.15	870.71
100.00	323.15	862.33
100.00	333.15	854.49
100.00	343.15	845.8
100.00	352.15	838.42
40000.00	280.15	914.37
40000.00	293.15	906.75
40000.00	303.15	895.63
40000.00	313.15	888.48
40000.00	323.15	881.75
40000.00	333.15	874.61

Reference *https://www.doi.org/10.1021/acs.jced.6b00360*

Sources

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Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester:	https://www.doi.org/10.1021/acs.jced.6b00360

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rhol:	Liquid Density
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