Nonadecanoic acid, methyl ester

Other names: Methyl nonadecanoate
methyl nonadecan-1-oate
n-Nonadecanoic acid methyl ester
Inchi: InChI=1S/C20H40O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-2/h3-19
InchiKey: BDXAHSJUDUZLDU-UHFFFAOYSA-N
Formula: C20H40O2
SMILES: CCCCCCCCCCCCCCCCCCC(=O)OC
Mol. weight [g/mol]: 312.53
CAS: 1731-94-8

Physical Properties

Property code	Value	Unit	Source
gf	-116.40	kJ/mol	Joback Method
hf	-700.93	kJ/mol	Joback Method
hfus	70.92	kJ/mol	Heat Capacity Measurements of 13 Methyl Esters of n-Carboxylic Acids from Methyloctanoate to Methyleicosanoate between 5 K and 350 K
hvap	109.50 ± 5.40	kJ/mol	NIST Webbook
hvap	109.50 ± 2.70	kJ/mol	NIST Webbook
log10ws	-7.06		Crippen Method
logp	6.811		Crippen Method
mcvol	300.100	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2204.90		NIST Webbook
rinpol	376.60		NIST Webbook
rinpol	376.70		NIST Webbook
rinpol	365.54		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2197.70		NIST Webbook
rinpol	2198.80		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2201.20		NIST Webbook

rinpol	2202.40		NIST Webbook
rinpol	2203.60		NIST Webbook
rinpol	365.43		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2211.00		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2226.20		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2221.00		NIST Webbook
rinpol	2209.00		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	365.43		NIST Webbook
ripol	2534.00		NIST Webbook
ripol	2543.00		NIST Webbook
ripol	2513.00		NIST Webbook
ripol	2539.00		NIST Webbook
tb	733.29	K	Joback Method
tc	904.52	K	Joback Method
tf	312.35 ± 0.40	K	NIST Webbook
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.52	J/mol×K	733.29	Joback Method
cpg	1013.17	J/mol×K	904.52	Joback Method
cpg	946.91	J/mol×K	790.37	Joback Method
cpg	964.76	J/mol×K	818.91	Joback Method
cpg	981.74	J/mol×K	847.45	Joback Method
cpg	997.86	J/mol×K	875.99	Joback Method
cpg	928.17	J/mol×K	761.83	Joback Method
dvisc	0.0000988	Pa×s	675.63	Joback Method
dvisc	0.0001407	Pa×s	617.97	Joback Method
dvisc	0.0002156	Pa×s	560.30	Joback Method
dvisc	0.0003644	Pa×s	502.64	Joback Method
dvisc	0.0007053	Pa×s	444.98	Joback Method

dvisc	0.0000733	Pa×s	733.29	Joback Method
dvisc	0.0016619	Pa×s	387.32	Joback Method
hfust	42.80	kJ/mol	313.20	NIST Webbook
hfust	63.80	kJ/mol	313.20	NIST Webbook
hfust	42.80	kJ/mol	313.20	NIST Webbook
hfust	19.40	kJ/mol	304.20	NIST Webbook
hvapt	90.10	kJ/mol	485.00	NIST Webbook
hvapt	105.00 ± 2.40	kJ/mol	326.00	NIST Webbook
hvapt	101.20	kJ/mol	350.00	NIST Webbook
sfust	63.70	J/mol×K	304.20	NIST Webbook
sfust	136.80	J/mol×K	313.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.02510e+01
Coeff. B	-7.76715e+03
Coeff. C	-1.28730e+02
Temperature range (K), min.	517.80
Temperature range (K), max.	648.64

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1731948&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume