

Nonadecanoic acid, ethyl ester

Other names:	ethyl nonadecanoate
Inchi:	InChI=1S/C21H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21(22)23-4-2/h3
InchiKey:	ICVYQLQYVCXJNE-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	326.56
CAS:	18281-04-4

Physical Properties

Property code	Value	Unit	Source
gf	-107.98	kJ/mol	Joback Method
hf	-721.57	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2282.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2274.00		NIST Webbook
ripol	2553.00		NIST Webbook
ripol	2559.00		NIST Webbook
ripol	2563.00		NIST Webbook
ripol	2565.00		NIST Webbook
ripol	2547.00		NIST Webbook
ripol	2547.00		NIST Webbook
tb	756.17	K	Joback Method
tc	929.77	K	Joback Method
tf	398.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.06	J/mol×K	871.90	Joback Method
cpg	1075.99	J/mol×K	929.77	Joback Method
cpg	1060.46	J/mol×K	900.83	Joback Method
cpg	969.32	J/mol×K	756.17	Joback Method
cpg	989.43	J/mol×K	785.10	Joback Method
cpg	1008.57	J/mol×K	814.04	Joback Method
cpg	1026.77	J/mol×K	842.97	Joback Method
dvisc	0.0000640	Pa×s	756.17	Joback Method
dvisc	0.0001235	Pa×s	636.98	Joback Method
dvisc	0.0000864	Pa×s	696.57	Joback Method
dvisc	0.0014949	Pa×s	398.59	Joback Method
dvisc	0.0006283	Pa×s	458.19	Joback Method
dvisc	0.0003224	Pa×s	517.78	Joback Method
dvisc	0.0001899	Pa×s	577.38	Joback Method
hfust	43.10	kJ/mol	309.00	NIST Webbook
hsubt	149.70	kJ/mol	305.00	NIST Webbook
hvapt	111.00	kJ/mol	320.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C18281044&Units=SI
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
hsubt:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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