Pentadecanoic acid, ethyl ester

Other names: Ethyl pentadecanoate
n-Pentadecanoic acid ethyl ester
Inchi: InChI=1S/C17H34O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19-4-2/h3-16H2,1-2H3
InchiKey: PTEYJUIKYIKULL-UHFFFAOYSA-N
Formula: C17H34O2
SMILES: CCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 270.45
CAS: 41114-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-141.66	kJ/mol	Joback Method
hf	-639.01	kJ/mol	Joback Method
hfus	42.57	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.641		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	1885.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1878.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1880.00		NIST Webbook
rinpol	1876.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1875.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1880.00		NIST Webbook

rinpol	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1893.00		NIST Webbook
rinpol	1877.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1885.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1876.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2140.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2146.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2157.00		NIST Webbook
ripol	2172.00		NIST Webbook
ripol	2179.00		NIST Webbook
ripol	2144.00		NIST Webbook
ripol	2116.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2126.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2135.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2161.00		NIST Webbook
ripol	2163.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2140.00		NIST Webbook
ripol	2172.00		NIST Webbook
tb	664.65	K	Joback Method
tc	832.26	K	Joback Method
tf	353.51	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	732.28	J/mol×K	664.65	Joback Method
cpg	750.62	J/mol×K	692.59	Joback Method
cpg	768.17	J/mol×K	720.52	Joback Method
cpg	784.95	J/mol×K	748.46	Joback Method
cpg	800.97	J/mol×K	776.39	Joback Method
cpg	816.25	J/mol×K	804.33	Joback Method
cpg	830.80	J/mol×K	832.26	Joback Method
dvisc	0.0022120	Pa×s	353.51	Joback Method
dvisc	0.0009695	Pa×s	405.37	Joback Method
dvisc	0.0005124	Pa×s	457.22	Joback Method
dvisc	0.0003083	Pa×s	509.08	Joback Method
dvisc	0.0002038	Pa×s	560.94	Joback Method
dvisc	0.0001445	Pa×s	612.79	Joback Method
dvisc	0.0001081	Pa×s	664.65	Joback Method

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=C41114005&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
hvap: Enthalpy of vaporization at standard conditions
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