Tetradecanoic acid, 1-methylethyl ester

Other names: 1-Tridecanecarboxylic acid, isopropyl ester
1-methylethyl tetradecanoate
Bisomel
Crodamol I.P.M.
Crodamol IPM
D 50
Deltyl Extra
Emcol-IM
Emerest 2314
Estergel
IPM
Isomyst
Ja-fa IPM
Kessco IPM
Kessco isopropyl myristate
Kesscomir
Lexol IPM
Liponate IPM
Methylethyl tetradecanoate
NSC 406280
Plymoutm IPM
Promyr
Radia 7190
Sinnoester MIP
Starfol IPM
Stepan D-50
Tegester
Tegosoft M
Tetradecanoic acid methyethyl ester
Tetradecanoic acid, isopropyl
Tetradecanoic acid, isopropyl ester
Unimate IPM
Wickenol 101
iso-Propyl N-tetradecanoate
isopropyl myristate
isopropyl tetradecanoate
myristic acid, isopropyl ester

Inchi: InChI=1S/C17H34O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-17(18)19-16(2)3/h16H,4-15H2,1

InchiKey: AXISYYRBXTVTFY-UHFFFAOYSA-N

Formula: C17H34O2

SMILES: CCCCCCCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]: 270.46
CAS: 110-27-0

Physical Properties

Property code	Value	Unit	Source
af	0.8332		Cheméo Relay (1.0)
hf	-730.94	kJ/mol	Cheméo Relay (1.0)
hfus	39.05	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Cheméo Relay (1.0)
ie	9.74	eV	Cheméo Relay (1.0)
log10ws	-5.87		Cheméo Relay (1.0)
logp	5.639		Crippen Method
mcvol	257.830	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1828.40		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1812.80		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1814.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1812.80		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1829.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1817.00		NIST Webbook
rinpol	1824.10		NIST Webbook

rinpol	1826.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1828.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1813.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1832.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2026.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2027.00		NIST Webbook
ripol	2023.00		NIST Webbook
tb	541.55	K	Cheméo Relay (1.0)
tc	729.56	K	Cheméo Relay (1.0)
tf	280.69	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.65	J/mol×K	805.55	Joback Method

cpg	832.34	J/mol×K	833.82	Joback Method
cpg	751.27	J/mol×K	692.48	Joback Method
cpg	769.05	J/mol×K	720.75	Joback Method
cpg	786.03	J/mol×K	749.02	Joback Method
cpg	802.22	J/mol×K	777.28	Joback Method
cpg	732.67	J/mol×K	664.21	Joback Method
dvisc	0.0005461	Pa×s	447.08	Joback Method
dvisc	0.0011177	Pa×s	392.79	Joback Method
dvisc	0.0028787	Pa×s	338.51	Joback Method
dvisc	0.0003116	Pa×s	501.36	Joback Method
dvisc	0.0001983	Pa×s	555.64	Joback Method
dvisc	0.0001368	Pa×s	609.93	Joback Method
dvisc	0.0001003	Pa×s	664.21	Joback Method
hvapt	70.20	kJ/mol	439.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	465.80	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68406e+01
Coeff. B	-5.83543e+03
Coeff. C	-1.09270e+02
Temperature range (K), min.	461.80
Temperature range (K), max.	615.42

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Solubility of the Antimicrobial Agent Triclosan in Organic Solvents of Different Hydrogen Bonding Capabilities at Several Temperatures: https://www.doi.org/10.1021/je800426w

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility of naproxen in several organic solvents at different temperatures:	https://www.doi.org/10.1016/j.fluid.2007.03.029
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C110270&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point