Isopropyl palmitate

Other names:	1-methylethyl hexadecanoate
	1-methylethyl hexandecanoate
	2-propyl hexadecanoate
	Crodamol IPP
	Deltyl
	Deltyl Prime
	Emcol-IP
	Emerest 2316
	Estol 103
	Hexadecanoic acid, 1-methylethyl ester
	Hexadecanoic acid, isopropyl ester
	Isopal
	Isopalm
	Isopropyl ester of hexadecanoic acid
	Isopropyl hexadecanoate
	Isopropyl n-hexadecanoate
	Ja-fa ipp
	Ja-fa ippkessco
	Kessco IPP
	Kessco isopropyl palmitate
	Lexol IPP
	Liponate IPP
	NSC 69169
	Nikkol IPP
	Palmitic acid, isopropyl ester
	Plymouth IPP
	Propal
	Radia 7200
	Sinnoester PIT
	Starfol IPP
	Stepan D-70
	Tegester isopalm
	Tegosoft P
	USAF KE-5
	Unimate IPP
	Wickenol 111
Inchi:	InChI=1S/C19H38O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-19(20)21-18(2)3/h18H,4-1
InchiKey:	XUGNVMKQXJXZCD-UHFFFAOYSA-N
Formula:	C19H38O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OC(C)C

Mol. weight [g/mol]: 298.50
CAS: 142-91-6

Physical Properties

Property code	Value	Unit	Source
gf	-127.26	kJ/mol	Joback Method
hf	-685.57	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.419		Crippen Method
mcvol	286.010	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2026.90		NIST Webbook
rinpol	2026.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2023.50		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	2027.00		NIST Webbook
rinpol	2011.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2232.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2232.00		NIST Webbook
tb	709.97	K	Joback Method
tc	880.96	K	Joback Method

tf	361.05	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.60	J/mol×K	880.96	Joback Method
cpg	937.44	J/mol×K	852.46	Joback Method
cpg	921.48	J/mol×K	823.96	Joback Method
cpg	904.69	J/mol×K	795.46	Joback Method
cpg	887.04	J/mol×K	766.97	Joback Method
cpg	868.53	J/mol×K	738.47	Joback Method
cpg	849.12	J/mol×K	709.97	Joback Method
dvisc	0.0023450	Pa×s	361.05	Joback Method
dvisc	0.0000774	Pa×s	709.97	Joback Method
dvisc	0.0001061	Pa×s	651.82	Joback Method
dvisc	0.0001546	Pa×s	593.66	Joback Method
dvisc	0.0002445	Pa×s	535.51	Joback Method
dvisc	0.0004323	Pa×s	477.36	Joback Method
dvisc	0.0008954	Pa×s	419.20	Joback Method
hvapt	73.60	kJ/mol	452.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.91779e+01
Coeff. B	-7.14651e+03
Coeff. C	-1.23004e+02
Temperature range (K), min.	501.32
Temperature range (K), max.	638.39

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C142916&Units=SI

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
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