Isopropyl stearate

Other names:	1-Methylethyl octadecanoate
	Octadecanoic acid, 1-methylethyl ester
	Octadecanoic acid, isopropyl ester
	Revenge
	Stearic acid, isopropyl ester
	Tegosoft S
	Wickenol 127
Inchi:	InChI=1S/C21H42O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20(2)3/h2
InchiKey:	ZPWFUIUNWDIYCJ-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OC(C)C
Mol. weight [g/mol]:	326.56
CAS:	112-10-7

Physical Properties

Property code	Value	Unit	Source
gf	-110.42	kJ/mol	Joback Method
hf	-726.85	kJ/mol	Joback Method
hfus	49.41	kJ/mol	Joback Method
hvap	71.11	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	7.200		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2217.00		NIST Webbook
tb	755.73	K	Joback Method
tc	930.28	K	Joback Method
tf	383.59	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.91	J/mol×K	930.28	Joback Method

cpg	969.75	J/mol×K	755.73	Joback Method
cpg	989.99	J/mol×K	784.82	Joback Method
cpg	1009.24	J/mol×K	813.91	Joback Method
cpg	1027.53	J/mol×K	843.00	Joback Method
cpg	1044.89	J/mol×K	872.09	Joback Method
cpg	1061.34	J/mol×K	901.19	Joback Method
dvisc	0.0000590	Pa×s	755.73	Joback Method
dvisc	0.0018724	Pa×s	383.59	Joback Method
dvisc	0.0007045	Pa×s	445.61	Joback Method
dvisc	0.0003366	Pa×s	507.64	Joback Method
dvisc	0.0001889	Pa×s	569.66	Joback Method
dvisc	0.0001187	Pa×s	631.68	Joback Method
dvisc	0.0000811	Pa×s	693.71	Joback Method
hvapt	76.60	kJ/mol	468.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.93960e+01
Coeff. B	-7.53425e+03
Coeff. C	-1.31510e+02
Temperature range (K), min.	525.80
Temperature range (K), max.	666.44

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112107&Units=SI

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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume