Octadecanoic acid, propyl ester

Other names:	Propyl octadecanoate
	Propyl stearate
	Stearic acid, propyl ester
Inchi:	InChI=1S/C21H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(22)23-20-4-2/h3
InchiKey:	BTAXGNQLYFDKEF-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCCC
Mol. weight [g/mol]:	326.56
CAS:	3634-92-2

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	2273.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2273.00		NIST Webbook
rinpol	2294.00		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	1075.99	J/mol×K	929.77	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
cpg	1044.06	J/mol×K	871.90	Joback Method
cpg	1060.46	J/mol×K	900.83	Joback Method
dvisc	0.0000640	Pa×s	756.17	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
dvisc	0.0001235	Pa×s	636.98	Joback Method
dvisc	0.0000864	Pa×s	696.57	Joback Method
hvapt	87.90	kJ/mol	470.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.96437e+01
Coeff. B	-7.73294e+03
Coeff. C	-1.34290e+02
Temperature range (K), min.	533.80
Temperature range (K), max.	673.84

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3634922&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