Octadecanoic acid, butyl ester

Other names:	ADK STAB LS-8
	Apex 4
	BS
	BUTYL ESTER
	Butyl octadecanoate
	Butyl stearate
	Emerest 2325
	Groco 5810
	Kemester 5510
	Kessco BS
	Kessco BSC
	Kesscoflex BS
	N-BUTYL OCTADECANOATE
	NSC 4820
	Oleo-Coll LP
	Oleoyl sarcosine
	Polycizer 332
	Priolube 1451
	RC Plasticizer B-17
	Radia 7051
	STEARIC ACID
	Starfol BS-100
	Stearic acid, butyl ester
	Tegester butyl stearate
	Uniflex BYS-tech
	Uniflex bys
	Unimate BYS
	Wickenol 122
	Witcizer 200
	Witcizer 201
	Witconol 2326
	n-Butyl stearate
Inchi:	InChI=1S/C22H44O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22(23)24-21-6-4-2
InchiKey:	ULBTUVJTXULMLP-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	340.58
CAS:	123-95-5

Physical Properties

Property code	Value	Unit	Source
chl	-13972.00	kJ/mol	NIST Webbook
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2388.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
tt	299.72 ± 0.02	K	NIST Webbook
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1139.78	J/mol×K	955.69	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1031.01	J/mol×K	779.05	Joback Method
cpg	1051.60	J/mol×K	808.49	Joback Method
cpg	1071.17	J/mol×K	837.93	Joback Method
cpg	1089.74	J/mol×K	867.37	Joback Method
dvisc	0.0001080	Pa×s	655.99	Joback Method

dvisc	0.0000754	Pa×s	717.52	Joback Method
dvisc	0.0000557	Pa×s	779.05	Joback Method
dvisc	0.0013386	Pa×s	409.86	Joback Method
dvisc	0.0005575	Pa×s	471.39	Joback Method
dvisc	0.0002843	Pa×s	532.92	Joback Method
dvisc	0.0001666	Pa×s	594.45	Joback Method
hfust	37.48	kJ/mol	299.70	NIST Webbook
hfust	37.48	kJ/mol	299.70	NIST Webbook
hfust	2.22	kJ/mol	288.40	NIST Webbook
hvapt	99.90	kJ/mol	375.50	NIST Webbook
sfust	125.05	J/mol×K	299.70	NIST Webbook
sfust	7.70	J/mol×K	288.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.03091e+01
Coeff. B	-8.19195e+03
Coeff. C	-1.39962e+02
Temperature range (K), min.	549.12
Temperature range (K), max.	686.18

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-3.21911e+01
Coeff. B	-9.32682e+03
Coeff. C	8.86661e+00
Coeff. D	-1.31917e-05
Temperature range (K), min.	299.45
Temperature range (K), max.	764.00

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Solubilities of n-Butyl Esters in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je500309x
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1136
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1136.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume