Oleic acid, butyl ester

Other names:	(Z)-9-Octadecenoic acid butyl ester
	9-Octadecenoic acid (9Z)-, butyl ester
	9-Octadecenoic acid (Z)-, butyl ester
	9-Octadecenoic acid, butyl ester (Z)-
	Advaplast 42
	Butyl 9-octadecenoate, cis-
	Butyl cis-9-octadecenoate
	Butyl oleate
	Emerest 2328
	Hallco C 503
	Hallco C-503 Plasticizer
	Kemester 4000
	Kessco 554
	Kesscoflex BO
	Plasthall 503
	Plasthall 914
	Uniflex byo
	Wilmar Butyl Oleate
	Witcizer 100
	Witcizer 101
	n-Butyl oleate
Inchi:	InChI=1S/C22H42O2/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:	WIBFFTLQMKKBLZ-SEYXRHQNSA-N
Formula:	C22H42O2
SMILES:	CCCCCCCCC=CCCCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	338.57
CAS:	142-77-8

Physical Properties

Property code	Value	Unit	Source
chl	-13843.00 ± 14.00	kJ/mol	NIST Webbook
gf	-19.34	kJ/mol	Joback Method
hf	-624.99	kJ/mol	Joback Method
hfus	55.72	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method

logp	7.367		Crippen Method
mcvol	323.980	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
tb	783.21	K	Joback Method
tc	962.10	K	Joback Method
tf	404.78	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.80	J/mol×K	962.10	Joback Method
cpg	1097.36	J/mol×K	932.29	Joback Method
cpg	1081.08	J/mol×K	902.47	Joback Method
cpg	1063.93	J/mol×K	872.66	Joback Method
cpg	1045.86	J/mol×K	842.84	Joback Method
cpg	1026.84	J/mol×K	813.03	Joback Method
cpg	1006.83	J/mol×K	783.21	Joback Method
dvisc	0.0012526	Pa×s	404.78	Joback Method
dvisc	0.0000483	Pa×s	783.21	Joback Method
dvisc	0.0000656	Pa×s	720.14	Joback Method
dvisc	0.0000943	Pa×s	657.07	Joback Method
dvisc	0.0001465	Pa×s	593.99	Joback Method
dvisc	0.0002528	Pa×s	530.92	Joback Method
dvisc	0.0005052	Pa×s	467.85	Joback Method
hvapt	97.70	kJ/mol	373.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45892e+01
Coeff. B	-6.95400e+03
Coeff. C	9.60200e+00
Temperature range (K), min.	476.64
Temperature range (K), max.	739.94

Sources

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=C142778&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

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