Octadecanoic acid, 2-methylpropyl ester

Other names:	Emerest 2324
	Estol 1476
	Isobutyl stearate
	Kemester 5415
	Kessco IBS
	Stearic acid, isobutyl ester
	Uniflex IBYS
Inchi:	InChI=1S/C22H44O2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(23)24-20-21(2)3
InchiKey:	ORFWYUFLWUWSFM-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	340.58
CAS:	646-13-9

Physical Properties

Property code	Value	Unit	Source
gf	-102.00	kJ/mol	Joback Method
hf	-747.49	kJ/mol	Joback Method
hfus	52.00	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	7.447		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	624.00 ± 6.00	K	NIST Webbook
tc	955.90	K	Joback Method
tf	394.86	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1031.45	J/mol×K	778.61	Joback Method
cpg	1124.73	J/mol×K	926.35	Joback Method
cpg	1108.04	J/mol×K	896.80	Joback Method
cpg	1090.39	J/mol×K	867.25	Joback Method
cpg	1071.76	J/mol×K	837.71	Joback Method
cpg	1052.12	J/mol×K	808.16	Joback Method
cpg	1140.50	J/mol×K	955.90	Joback Method
dvisc	0.0000512	Pa×s	778.61	Joback Method
dvisc	0.0000706	Pa×s	714.65	Joback Method
dvisc	0.0001035	Pa×s	650.69	Joback Method
dvisc	0.0001652	Pa×s	586.74	Joback Method
dvisc	0.0002954	Pa×s	522.78	Joback Method
dvisc	0.0006213	Pa×s	458.82	Joback Method
dvisc	0.0016625	Pa×s	394.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.02025e+01
Coeff. B	-8.06428e+03
Coeff. C	-1.37182e+02
Temperature range (K), min.	542.12
Temperature range (K), max.	678.74

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C646139&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
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