Butyric acid, octadecyl ester

Other names:	Butanoic acid, octadecyl ester
	Octadecyl butanoate
	Octadecyl butyrate
Inchi:	InChI=1S/C22H44O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21-24-22(23)20-4-2
InchiKey:	VTTIDPAZLXIGNF-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCCCOC(=O)CCC
Mol. weight [g/mol]:	340.58
CAS:	13373-83-6

Physical Properties

Property code	Value	Unit	Source
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	2362.00		NIST Webbook
rinpol	2363.00		NIST Webbook
rinpol	2352.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2363.00		NIST Webbook
ripol	2595.00		NIST Webbook
ripol	2595.00		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	1107.35	J/mol×K	896.81	Joback Method
cpg	1124.02	J/mol×K	926.25	Joback Method
cpg	1139.78	J/mol×K	955.69	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
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.24916e+01
Coeff. B	-9.10717e+03
Coeff. C	-1.39962e+02
Temperature range (K), min.	550.12
Temperature range (K), max.	670.06

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13373836&Units=SI

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