Tributyrin

Other names:	1,2,3-Propanetriol, tributyrate
	1,2,3-propanetriyl tributanoate
	Butanoic acid, 1,2,3-propanetriyl ester
	Butyric acid triester with glycerin
	Butyrin
	Butyrin, tri-
	Butyryl triglyceride
	Glycerin tributyrate
	Glycerol tributyrate
	Glyceroltributyrin
	NSC 661583
	Tri-n-butyrin
	Tributin
	Tributyroin
	Tributyryl glyceride
	glycerol tributanoate
	glyceryl tributyrate
	propane-1,2,3-triyl tributyrate
	tributyrylglycerol
Inchi:	InChI=1S/C15H26O6/c1-4-7-13(16)19-10-12(21-15(18)9-6-3)11-20-14(17)8-5-2/h12H,4-1
InchiKey:	UYXTWWCETRIEDR-UHFFFAOYSA-N
Formula:	C15H26O6
SMILES:	CCCC(=O)OCC(COC(=O)CCC)OC(=O)CCC
Mol. weight [g/mol]:	302.36
CAS:	60-01-5

Physical Properties

Property code	Value	Unit	Source
chl	-8122.40	kJ/mol	NIST Webbook
gf	-628.78	kJ/mol	Joback Method
hf	-1092.61	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	107.10 ± 1.00	kJ/mol	NIST Webbook
hvap	107.10 ± 1.00	kJ/mol	NIST Webbook
hvap	84.90 ± 2.50	kJ/mol	NIST Webbook
hvap	107.07	kJ/mol	NIST Webbook
log10ws	-2.80		Crippen Method

logp	2.385		Crippen Method
mcvol	244.530	ml/mol	McGowan Method
pc	1584.75	kPa	Joback Method
rinpol	1813.00		NIST Webbook
rinpol	1815.00		NIST Webbook
rinpol	1816.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	580.70	K	NIST Webbook
tc	957.68	K	Joback Method
tf	460.29	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.57	J/mol×K	771.03	Joback Method
cpg	743.38	J/mol×K	802.14	Joback Method
cpg	757.29	J/mol×K	833.25	Joback Method
cpg	770.29	J/mol×K	864.36	Joback Method
cpg	782.38	J/mol×K	895.47	Joback Method
cpg	793.56	J/mol×K	926.57	Joback Method
cpg	803.82	J/mol×K	957.68	Joback Method
cpl	555.30	J/mol×K	298.15	NIST Webbook
cpl	569.00	J/mol×K	313.00	NIST Webbook
dvisc	0.0008806	Pa×s	460.29	Joback Method
dvisc	0.0004692	Pa×s	512.08	Joback Method
dvisc	0.0002806	Pa×s	563.87	Joback Method
dvisc	0.0001830	Pa×s	615.66	Joback Method
dvisc	0.0001275	Pa×s	667.45	Joback Method
dvisc	0.0000936	Pa×s	719.24	Joback Method
dvisc	0.0000716	Pa×s	771.03	Joback Method
hvapt	83.50	kJ/mol	308.00	NIST Webbook
hvapt	81.40	kJ/mol	341.00	NIST Webbook
pvap	1.69	kPa	459.56	Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	474.55	K	3.47	Improving a variation of the DSC technique for measuring the boiling points of pure compounds at low pressures
tbrp	463.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60015&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of CO2 in triglycerides using Monte Carlo simulations:	https://www.doi.org/10.1016/j.fluid.2018.01.003
Improving a variation of the DSC technique for measuring the boiling points of pure compounds at low pressures:	https://www.doi.org/10.1016/j.jct.2016.04.023
Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures:	https://www.doi.org/10.1021/acs.jced.8b00168
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume