1,2,3-Propanetricarboxylic acid, 2-(acetyloxy)-, tris(2-ethylhexyl) ester

Other names:	O-Acetyl tris(2-ethylhexyl)citrate
	Acetyl-tris-(2-ethylhexyl) citrate
	Citric acid, tris[2-ethylhexyl] ester, acetate
	tris(2-ethylhexyl) 2-(acetyloxy)propane-1,2,3-tricarboxylate
Inchi:	InChI=1S/C32H58O8/c1-8-14-17-26(11-4)22-37-29(34)20-32(40-25(7)33,31(36)39-24-28
InchiKey:	FRDNONBEXWDRDM-UHFFFAOYSA-N
Formula:	C32H58O8
SMILES:	CCCCC(CC)COC(=O)CC(CC(=O)OCC(CC)CCCC)(OC(C)=O)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	570.80
CAS:	144-15-0

Physical Properties

Property code	Value	Unit	Source
gf	-721.60	kJ/mol	Joback Method
hf	-1707.60	kJ/mol	Joback Method
hfus	71.80	kJ/mol	Joback Method
hvap	120.99	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.347		Crippen Method
mcvol	491.500	ml/mol	McGowan Method
pc	605.77	kPa	Joback Method
tb	1232.17	K	Joback Method
tc	1596.89	K	Joback Method
tf	696.46	K	Joback Method
vc	1.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1804.53	J/mol×K	1232.17	Joback Method
cpg	1818.04	J/mol×K	1292.96	Joback Method
cpg	1826.64	J/mol×K	1353.74	Joback Method
cpg	1830.58	J/mol×K	1414.53	Joback Method
cpg	1830.12	J/mol×K	1475.31	Joback Method

cpg	1825.51	J/mol×K	1536.10	Joback Method
cpg	1816.99	J/mol×K	1596.89	Joback Method
dvisc	0.0000477	Pa×s	696.46	Joback Method
dvisc	0.0000206	Pa×s	785.74	Joback Method
dvisc	0.0000105	Pa×s	875.03	Joback Method
dvisc	0.0000061	Pa×s	964.32	Joback Method
dvisc	0.0000039	Pa×s	1053.60	Joback Method
dvisc	0.0000027	Pa×s	1142.88	Joback Method
dvisc	0.0000019	Pa×s	1232.17	Joback Method

Sources

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=C144150&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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