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	1825.51	J/mol×K	1536.10	Joback Method
cpg	1830.12	J/mol×K	1475.31	Joback Method
cpg	1830.58	J/mol×K	1414.53	Joback Method
cpg	1826.64	J/mol×K	1353.74	Joback Method

cpg	1818.04	J/mol×K	1292.96	Joback Method
cpg	1816.99	J/mol×K	1596.89	Joback Method
dvisc	0.0000019	Pa×s	1232.17	Joback Method
dvisc	0.0000027	Pa×s	1142.88	Joback Method
dvisc	0.0000039	Pa×s	1053.60	Joback Method
dvisc	0.0000061	Pa×s	964.32	Joback Method
dvisc	0.0000105	Pa×s	875.03	Joback Method
dvisc	0.0000206	Pa×s	785.74	Joback Method
dvisc	0.0000477	Pa×s	696.46	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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