ACETYL TRIS(2-ETHYLHEXYL)CITRATE

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]:	570.81

Physical Properties

Property code	Value	Unit	Source
hfus	71.80	kJ/mol	Joback Method
log10ws	-7.03		Cheméo Relay (1.0)
logp	7.347		Crippen Method
mcvol	491.500	ml/mol	McGowan Method
pc	605.77	kPa	Joback Method
tb	708.88	K	Cheméo Relay (1.0)
tf	248.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1804.53	J/mol×K	1232.17	Joback Method
cpg	1816.99	J/mol×K	1596.89	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
dvisc	0.0000061	Pa×s	964.32	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	0.0000477	Pa×s	696.46	Joback Method
dvisc	0.0000105	Pa×s	875.03	Joback Method
dvisc	0.0000206	Pa×s	785.74	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C144150&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion 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
tf: Normal melting (fusion) point