

Stearic acid, triethylcitrate ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C30H54O8/c1-5-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-26(31)38-30(2

CPWUFKKGVRVSNX-UHFFFAOYSA-N

C30H54O8

CCCCCCCCCCCCCCCCCCCC(=O)OC(CC(=O)OCC)(CC(=O)OCC)C(=O)OCC

542.75

Physical Properties

Property code	Value	Unit	Source
gf	-731.12	kJ/mol	Joback Method
hf	-1650.48	kJ/mol	Joback Method
hfus	77.19	kJ/mol	Joback Method
hvap	117.70	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.999		Crippen Method
mcvol	463.320	ml/mol	McGowan Method
pc	659.15	kPa	Joback Method
tb	1187.73	K	Joback Method
tc	1526.42	K	Joback Method
tf	718.92	K	Joback Method
vc	1.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1681.18	J/mol×K	1187.73	Joback Method
cpg	1696.31	J/mol×K	1244.18	Joback Method
cpg	1707.26	J/mol×K	1300.63	Joback Method
cpg	1714.21	J/mol×K	1357.07	Joback Method
cpg	1717.33	J/mol×K	1413.52	Joback Method
cpg	1716.81	J/mol×K	1469.97	Joback Method
cpg	1712.80	J/mol×K	1526.42	Joback Method
dvisc	0.0000526	Pa×s	718.92	Joback Method
dvisc	0.0000272	Pa×s	797.06	Joback Method
dvisc	0.0000158	Pa×s	875.19	Joback Method

dvisc	0.0000100	Pa×s	953.33	Joback Method
dvisc	0.0000068	Pa×s	1031.46	Joback Method
dvisc	0.0000049	Pa×s	1109.60	Joback Method
dvisc	0.0000037	Pa×s	1187.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007398&Units=SI
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

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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