

(«beta»-acetoxy-octadecanoyl)-acetyl-glycerol

Inchi:	InChI=1S/C27H48O8/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25(34-23(3)29)19-27(31
InchiKey:	UWEMKTDDCINNINX-UHFFFAOYSA-N
Formula:	C27H48O8
SMILES:	CCCCCCCCCCCCCCCC(CC(=O)OCC(COC(C)=O)OC(C)=O)OC(C)=O
Mol. weight [g/mol]:	500.67

Physical Properties

Property code	Value	Unit	Source
gf	-764.10	kJ/mol	Joback Method
hf	-1590.37	kJ/mol	Joback Method
hfus	69.79	kJ/mol	Joback Method
hvap	111.54	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.828		Crippen Method
mcvol	421.050	ml/mol	McGowan Method
pc	767.34	kPa	Joback Method
rinpol	2910.00		NIST Webbook
tb	1121.44	K	Joback Method
tc	1410.37	K	Joback Method
tf	652.69	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1494.32	J/molxK	1121.44	Joback Method
cpg	1508.33	J/molxK	1169.60	Joback Method
cpg	1518.88	J/molxK	1217.75	Joback Method
cpg	1526.02	J/molxK	1265.91	Joback Method
cpg	1529.78	J/molxK	1314.06	Joback Method
cpg	1530.20	J/molxK	1362.22	Joback Method
cpg	1527.32	J/molxK	1410.37	Joback Method
dvisc	0.0001149	Paxs	652.69	Joback Method
dvisc	0.0000559	Paxs	730.82	Joback Method

dvisc	0.0000312	Paxs	808.94	Joback Method
dvisc	0.0000193	Paxs	887.07	Joback Method
dvisc	0.0000129	Paxs	965.19	Joback Method
dvisc	0.0000092	Paxs	1043.32	Joback Method
dvisc	0.0000069	Paxs	1121.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R277731&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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