

Glyceryl tri-18-acetoxystearate

Inchi: InChI=1S/C63H116O12/c1-57(64)70-52-46-40-34-28-22-16-10-4-7-13-19-25-31-37-43-49
InchiKey: GKLLDHHZSUEWRE-UHFFFAOYSA-N
Formula: C63H116O12
SMILES: CC(=O)OCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCCO)OCC(=O)OCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]: 1065.59

Physical Properties

Property code	Value	Unit	Source
gf	-926.38	kJ/mol	Joback Method
hf	-2817.73	kJ/mol	Joback Method
hfus	172.12	kJ/mol	Joback Method
hvap	210.38	kJ/mol	Joback Method
log10ws	-19.48		Crippen Method
logp	17.399		Crippen Method
mcvol	943.170	ml/mol	McGowan Method
pc	205.14	kPa	Joback Method
tb	2098.14	K	Joback Method
tf	1217.73	K	Joback Method
vc	3.701	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3278.67	J/molxK	2098.14	Joback Method
dvisc	9.2904573e-08	Paxs	1217.73	Joback Method
dvisc	2.3989895e-08	Paxs	1511.20	Joback Method
dvisc	1.4591040e-08	Paxs	1657.93	Joback Method
dvisc	9.6218819e-09	Paxs	1804.67	Joback Method
dvisc	6.7550424e-09	Paxs	1951.40	Joback Method
dvisc	4.9829309e-09	Paxs	2098.14	Joback Method
dvisc	4.3895035e-08	Paxs	1364.47	Joback Method

Sources

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=B6009643&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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