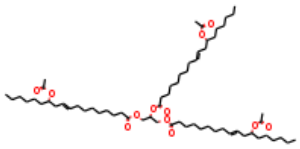
Glyceryl tri(acetylricinoleate)



Other names: 1,2,3-propanetriyl tris[(R)-12-(acetoxy)oleate].

InChI: InChI=1S/C63H110O12/c1-7-10-13-34-43-57(72-54(4)64)46-37-28-22-16-19-25-31-40-49-61(67)70-52-60(75-63(69)51-42-33-27-21-18-24-30-39-48-59(74-56(6)66)45-36-15-12-9-3)53-71-62(68)50-41-32-26-20-17-23-29-38-47-58(73-55(5)65)44-35-14-11-8-2/h28-30,37-39,57-60H,7-27,31-36,40-53H2,1-6H3/b37-28+,38-29+,39-30+

InChI Key: RIXCYAQOGLLEIU-OTDRRXFESA-N

Formula: C63H110O12

SMILES: CCCCCCC(CC=CCCCCCCCC(=O)OCC(COC(=O)CCCCCCCC=CCC(CCCCCC)OC(C)=O)OC(=O)CCCCCCCC=CCC(CCCCCC)OC(C)=O)OC(C)=O

Molecular Weight: 1059.54

CAS: 101-34-8

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-693.04	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-2481.91	kJ/mol	Joback Method
$\Delta_{fus} H°$	162.16	kJ/mol	Joback Method
$\Delta_{vap} H°$	209.09	kJ/mol	Joback Method
$logP_{oct/wat}$	16.72		Crippen Method
P_c	216.14	kPa	Joback Method
T_{boil}	2109.30	K	Joback Method
T_c	21893.24	K	Joback Method
T_{fus}	1157.49	K	Joback Method
V_c	3.62	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	3544.26	J/mol×K	2109.3	Joback Method
η	0.00	Pa×s	2109.3	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C63H110O12/c1-7-10-13-34-43-57(72-54(4)64)46-37-28-22-16-19-25-31-40-49-61(67)70-52-60(75-63(69)51-42-33-27-21-18-24-30-39-48-59(74-56(66)66)45-36-15-12-9-3)53-71-62(68)50-41-32-26-20-17-23-29-38-47-58(73-55(5)65)44-35-14-11-8-2/h28-30,37-39,57-60H,7-27,31-36,40-53H2,1-6H3/b37-28+,38-29+,39-30+

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).