9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester

Other names: Glyceryl Monooleate
Olein, 1-mono-
«alpha»-Monoolein
Aldo HMO
Aldo MO
Glycerin 1-monooleate
Glycerol «alpha»-cis-9-octadecenate
Glycerol «alpha»-monooleate
Glycerol 1-monooleate
Monoolein
1-Glyceryl oleate
1-Monoolein
1-Monooleoylglycerol
1-Oleoylglycerol
1-Oleylglycerol
dl-«alpha»-Monoolein
1-Monooleoyl-rac-glycerol
Ablunol GMO
Glycerol-1-oleate
Glycerol oleate
Glyceryl oleate
Witconol 2421
9-Octadecenoic acid (9Z)-, 2,3-dihydroxypropyl ester
1-Mono(cis-9-octacenoyl)glycerol
2,3-Dihydroxypropyl oleate
Danisco MO 90
rac-1-Monoolein
rac-1-Monooleoylglycerol
2,3-Dihydroxypropyl (9z)-9-octadecenoate

Inchi: InChI=1S/C21H40O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-19-20(23)18

InchiKey: RZRNAYUHWVFMIP-KTKRTIGZSA-N

Formula: C21H40O4

SMILES: CCCCCCCCC=CCCCCCCCC(=O)OCC(O)CO

Mol. weight [g/mol]: 356.54

CAS: 111-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-303.84	kJ/mol	Joback Method
hf	-914.09	kJ/mol	Joback Method
hfus	57.79	kJ/mol	Joback Method
hvap	104.42	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.920		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	944.25	K	Joback Method
tc	1164.97	K	Joback Method
tf	500.15	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.02	J/mol×K	944.25	Joback Method
cpg	1108.83	J/mol×K	981.04	Joback Method
cpg	1125.49	J/mol×K	1017.82	Joback Method
cpg	1141.06	J/mol×K	1054.61	Joback Method
cpg	1155.62	J/mol×K	1091.40	Joback Method
cpg	1169.25	J/mol×K	1128.19	Joback Method
cpg	1182.01	J/mol×K	1164.97	Joback Method
dvisc	0.0002857	Pa×s	500.15	Joback Method
dvisc	0.0000592	Pa×s	574.17	Joback Method
dvisc	0.0000176	Pa×s	648.18	Joback Method
dvisc	0.0000067	Pa×s	722.20	Joback Method
dvisc	0.0000030	Pa×s	796.22	Joback Method
dvisc	0.0000016	Pa×s	870.23	Joback Method
dvisc	0.0000009	Pa×s	944.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111035&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume