9-Octadecenoic acid, 12-(acetyloxy)-, methyl ester, [R-(Z)]-

Other names: Ricinoleic acid, methyl ester, acetate
Flexricin P-4
Methyl acetyl ricinoleate
Methyl ricinoleate, acetate
Methyl 12-acetoxyoleate
Methyl 12-acetoxy-9-octadecenoate
Methylester kyseliny acetylricinolejove
Naturechem MAR
Methyl (9Z)-12-(acetyloxy)-9-octadecenoate, (R)-
9-Octadecenoic acid, 12-acetoxy-, [R-(Z)], methyl ester
9-Octadecenoic acid, 12-(acetyloxy)-, methyl ester, (9Z,12R)-
NSC 2398
MAR-N
METHYL (R)-CIS-12-ACETOXY-9-OCTADECENOATE
9-Octadecenoic acid, d-12-acetoxy-, (z), methyl ester
methyl O-acetylricinoleate

Inchi: InChI=1S/C21H38O4/c1-4-5-6-13-16-20(25-19(2)22)17-14-11-9-7-8-10-12-15-18-21(23)2

InchiKey: CMOYPQWMTBSLJK-QKQONQEDSA-N

Formula: C21H38O4

SMILES: CCCCCCC(CC=CCCCCCCCC(=O)OC)OC(C)=O

Mol. weight [g/mol]: 354.52

CAS: 140-03-4

Physical Properties

Property code	Value	Unit	Source
gf	-264.12	kJ/mol	Joback Method
hf	-854.43	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	80.22	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.739		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1052.77	kPa	Joback Method
tb	836.18	K	Joback Method
tc	1026.01	K	Joback Method
tf	450.67	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.95	J/mol×K	836.18	Joback Method
cpg	1023.11	J/mol×K	867.82	Joback Method
cpg	1040.19	J/mol×K	899.46	Joback Method
cpg	1056.24	J/mol×K	931.09	Joback Method
cpg	1071.28	J/mol×K	962.73	Joback Method
cpg	1085.33	J/mol×K	994.37	Joback Method
cpg	1098.44	J/mol×K	1026.01	Joback Method
dvisc	0.0008233	Pa×s	450.67	Joback Method
dvisc	0.0003550	Pa×s	514.92	Joback Method
dvisc	0.0001845	Pa×s	579.17	Joback Method
dvisc	0.0001092	Pa×s	643.42	Joback Method
dvisc	0.0000712	Pa×s	707.68	Joback Method
dvisc	0.0000498	Pa×s	771.93	Joback Method
dvisc	0.0000368	Pa×s	836.18	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=C140034&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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