2,4-Octadienoic acid, 7-hydroxy-, methyl ester, [R-(E,E)]-

Other names: Methyl (2E,4E)-7-hydroxy-2,4-octadienoate
Methyl 2,4-octadienoic acid, 7-hydroxy-, [R-(E,E)]-
methyl 2,4-octadienoic acid, 7-hydroxy-

Inchi: InChI=1S/C9H14O3/c1-8(10)6-4-3-5-7-9(11)12-2/h3-5,7-8,10H,6H2,1-2H3/b4-3+,7-5+

InchiKey: VOFUNAIXXYFZAG-BDWKERMESA-N

Formula: C9H14O3

SMILES: COC(=O)C=CC=CCC(C)O

Mol. weight [g/mol]: 170.21

CAS: 69734-24-3

Physical Properties

Property code	Value	Unit	Source
gf	-187.84	kJ/mol	Joback Method
hf	-396.96	kJ/mol	Joback Method
hfus	22.82	kJ/mol	Joback Method
hvap	60.99	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.043		Crippen Method
mcvol	142.380	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1455.00		NIST Webbook
tb	581.67	K	Joback Method
tc	765.43	K	Joback Method
tf	299.01	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.81	J/mol×K	581.67	Joback Method
cpg	351.58	J/mol×K	612.30	Joback Method
cpg	361.81	J/mol×K	642.92	Joback Method
cpg	371.52	J/mol×K	673.55	Joback Method
cpg	380.74	J/mol×K	704.18	Joback Method

cpg	389.50	J/mol×K	734.80	Joback Method
cpg	397.81	J/mol×K	765.43	Joback Method
dvisc	0.0116386	Pa×s	299.01	Joback Method
dvisc	0.0026679	Pa×s	346.12	Joback Method
dvisc	0.0008704	Pa×s	393.23	Joback Method
dvisc	0.0003609	Pa×s	440.34	Joback Method
dvisc	0.0001774	Pa×s	487.45	Joback Method
dvisc	0.0000988	Pa×s	534.56	Joback Method
dvisc	0.0000605	Pa×s	581.67	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69734243&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

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