2-Octenoic acid, 4-isopropylidene-7-methyl-6-methylene-, methyl ester

Other names: 4-Isopropylidene-7-methyl-6-methylene-2-octenoic acid, methyl ester

Inchi: InChI=1S/C14H22O2/c1-10(2)12(5)9-13(11(3)4)7-8-14(15)16-6/h7-8,10H,5,9H2,1-4,6H3/

InchiKey: DADDHWNPTKGIBN-BQYQJAHWSA-N

Formula: C14H22O2

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

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	53.27	kJ/mol	Joback Method
hf	-251.87	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	55.01	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.654		Crippen Method
mcvol	202.660	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
tb	600.21	K	Joback Method
tc	795.55	K	Joback Method
tf	250.90	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.94	J/mol×K	600.21	Joback Method
cpg	522.52	J/mol×K	632.77	Joback Method
cpg	538.22	J/mol×K	665.32	Joback Method
cpg	553.09	J/mol×K	697.88	Joback Method
cpg	567.17	J/mol×K	730.44	Joback Method
cpg	580.51	J/mol×K	763.00	Joback Method
cpg	593.14	J/mol×K	795.55	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151992&Units=SI

Legend

cpg:	Ideal gas heat capacity
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