

1-Cyclohexene-1-carboxylic acid, 4-(1,5-dimethyl-3-oxo-4-hexenyl)-, methyl ester, [R-(R*)]-

Other names:	(+)-methyl 4'-Dehydrojuvabione Dehydrojuvabione Juvabione, dehydro- 1-Cyclohexene-1-carboxylic acid, 4-(1,5-dimethyl-3-oxo-4-hexenyl)-, methyl ester
Inchi:	InChI=1S/C16H24O3/c1-11(2)9-15(17)10-12(3)13-5-7-14(8-6-13)16(18)19-4/h7,9,12-13H
InchiKey:	DEMNMQDWPCIOLA-UHFFFAOYSA-N
Formula:	C16H24O3
SMILES:	COC(=O)C1=CCC(C(C)CC(=O)C=C(C(C)C)CC1
Mol. weight [g/mol]:	264.36
CAS:	16060-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-164.99	kJ/mol	Joback Method
hf	-528.17	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.447		Crippen Method
mcvol	225.850	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2089.00		NIST Webbook
tb	722.93	K	Joback Method
tc	934.92	K	Joback Method
tf	378.79	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.55	J/mol×K	722.93	Joback Method
cpg	668.41	J/mol×K	758.26	Joback Method
cpg	685.13	J/mol×K	793.59	Joback Method
cpg	700.73	J/mol×K	828.93	Joback Method

cpg	715.25	J/mol×K	864.26	Joback Method
cpg	728.74	J/mol×K	899.59	Joback Method
cpg	741.23	J/mol×K	934.92	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=C16060789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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