2,4-Pentadienoic acid, 5-(1-hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1 methyl ester, (R)-(Z,E)-

Other names: Methyl abscisate

Inchi: InChI=1S/C16H22O4/c1-11(8-14(18)20-5)6-7-16(19)12(2)9-13(17)10-15(16,3)4/h6-9,19H

InchiKey: HHDYPZVHXGPCRG-XSMWWFTRSA-N

Formula: C16H22O4

SMILES: COC(=O)C=C(C)C=CC1(O)C(C)=CC(=O)CC1(C)C

Mol. weight [g/mol]: 278.34

CAS: 7200-31-9

Physical Properties

Property code	Value	Unit	Source
gf	-231.51	kJ/mol	Joback Method
hf	-572.88	kJ/mol	Joback Method
hfus	23.82	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.338		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2112.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	829.47	K	Joback Method
tc	1049.82	K	Joback Method
tf	511.38	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.10	J/mol×K	829.47	Joback Method
cpg	713.78	J/mol×K	866.20	Joback Method
cpg	731.59	J/mol×K	902.92	Joback Method

cpg	749.72	J/mol×K	939.65	Joback Method
cpg	768.36	J/mol×K	976.37	Joback Method
cpg	787.72	J/mol×K	1013.10	Joback Method
cpg	807.99	J/mol×K	1049.82	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=C7200319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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