2,4-Pentadienoic acid, 5-(8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-, [1R-[1«alpha»,5«alpha»,8S*(2Z,4E)]]-

Other names:	2,4-Pentadienoic acid, 5-(8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl- Phaseic acid 2,4-Pentadienoic acid, 5-(8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-, [1R-[1«alpha»,5«alpha»,8S*(Z,E)]]- 6-Oxabicyclo[3.2.1]octane-2,4-pentadienoic acid deriv. Me-phaseic acid
Inchi:	InChI=1S/C15H20O5/c1-10(6-12(17)18)4-5-15(19)13(2)7-11(16)8-14(15,3)20-9-13/h4-6,
InchiKey:	IZGYIFFQBZWOLJ-UMCKCUICSA-N
Formula:	C15H20O5
SMILES:	CC(C=CC1(O)C2(C)COC1(C)CC(=O)C2)=CC(=O)O
Mol. weight [g/mol]:	280.32
CAS:	24394-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-310.84	kJ/mol	Joback Method
hf	-656.36	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	94.25	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.463		Crippen Method
mcvol	212.640	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
rinpol	2094.00		NIST Webbook
rinpol	2094.00		NIST Webbook
tb	901.87	K	Joback Method
tc	1124.91	K	Joback Method
tf	597.35	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.78	J/mol×K	901.87	Joback Method
cpg	730.53	J/mol×K	939.04	Joback Method

cpg	753.00	J/mol×K	976.22	Joback Method
cpg	777.56	J/mol×K	1013.39	Joback Method
cpg	804.55	J/mol×K	1050.56	Joback Method
cpg	834.34	J/mol×K	1087.74	Joback Method
cpg	867.28	J/mol×K	1124.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24394147&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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