Methyl phaseate

Other names:	2,4-Pentadienoic acid, 5-(8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-, methyl ester, [1R-[1«alpha»,5«alpha»,8S*(2Z,4E)]]- 2,4-Pentadienoic acid, 5-(8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl-, methyl ester, [1R-[1«alpha»,5«alpha»,8S*(Z,E)]]- Methyl (2Z,4E)-5-(1R,5R,8S)-8-hydroxy-1,5-dimethyl-3-oxo-6-oxabicyclo[3.2.1]oct-8-yl)-3-methyl Phaseic acid methyl ester Me-2-trans-phaseic acid
Inchi:	InChI=1S/C16H22O5/c1-11(7-13(18)20-4)5-6-16(19)14(2)8-12(17)9-15(16,3)21-10-14/h5
InchiKey:	BGXJFSPEUCRBIH-LCAICKDSSA-N
Formula:	C16H22O5
SMILES:	COC(=O)C=C(C)C=CC1(O)C2(C)COC1(C)CC(=O)C2
Mol. weight [g/mol]:	294.34
CAS:	41670-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-270.60	kJ/mol	Joback Method
hf	-656.99	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Joback Method
hvap	82.21	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.551		Crippen Method
mcvol	226.730	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	2154.00		NIST Webbook
tb	854.99	K	Joback Method
tc	1083.29	K	Joback Method
tf	570.03	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.62	J/mol×K	854.99	Joback Method
cpg	754.27	J/mol×K	893.04	Joback Method
cpg	776.11	J/mol×K	931.09	Joback Method

cpg	799.51	J/mol×K	969.14	Joback Method
cpg	824.82	J/mol×K	1007.19	Joback Method
cpg	852.41	J/mol×K	1045.24	Joback Method
cpg	882.66	J/mol×K	1083.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41670488&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
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