

# epi-Me-dihydrophaseic acid-Ac

<b>Inchi:</b>	InChI=1S/C18H26O6/c1-12(8-15(20)22-5)6-7-18(21)16(3)9-14(24-13(2)19)10-17(18,4)23
<b>InchiKey:</b>	ONGJVIGGHJEDKU-IWPPBABSSA-N
<b>Formula:</b>	C18H26O6
<b>SMILES:</b>	<chem>COC(=O)C=C(C)C=CC1(O)C2(C)COC1(C)CC(OC(C)=O)C2</chem>
<b>Mol. weight [g/mol]:</b>	338.40

## Physical Properties

Property code	Value	Unit	Source
gf	-372.80	kJ/mol	Joback Method
hf	-825.71	kJ/mol	Joback Method
hfus	34.43	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.914		Crippen Method
mcvol	260.780	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinsol	2247.00		NIST Webbook
tb	904.55	K	Joback Method
tc	1125.11	K	Joback Method
tf	592.27	K	Joback Method
vc	0.983	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.85	J/mol×K	904.55	Joback Method
cpg	898.01	J/mol×K	941.31	Joback Method
cpg	922.61	J/mol×K	978.07	Joback Method
cpg	948.97	J/mol×K	1014.83	Joback Method
cpg	977.45	J/mol×K	1051.59	Joback Method
cpg	1008.38	J/mol×K	1088.35	Joback Method
cpg	1042.12	J/mol×K	1125.11	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R487379&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R487379&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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