

# Me-2-trans-dihydrophaseic acid

<b>Inchi:</b>	InChI=1S/C16H24O5/c1-11(7-13(18)20-4)5-6-16(19)14(2)8-12(17)9-15(16,3)21-10-14/h5
<b>InchiKey:</b>	QNMHUZMKLBWTQM-PSCDLIPDSA-N
<b>Formula:</b>	C16H24O5
<b>SMILES:</b>	<chem>COC(=O)C=C(C)C=CC1(O)C2(C)COC1(C)CC(O)C2</chem>
<b>Mol. weight [g/mol]:</b>	296.36

## Physical Properties

Property code	Value	Unit	Source
gf	-292.54	kJ/mol	Joback Method
hf	-691.86	kJ/mol	Joback Method
hfus	30.55	kJ/mol	Joback Method
hvap	94.33	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.343		Crippen Method
mvol	231.030	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook
tb	874.68	K	Joback Method
tc	1086.40	K	Joback Method
tf	558.39	K	Joback Method
vc	0.866	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.50	J/mol×K	874.68	Joback Method
cpg	788.53	J/mol×K	909.97	Joback Method
cpg	809.81	J/mol×K	945.25	Joback Method
cpg	832.67	J/mol×K	980.54	Joback Method
cpg	857.42	J/mol×K	1015.82	Joback Method
cpg	884.38	J/mol×K	1051.11	Joback Method
cpg	913.86	J/mol×K	1086.40	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R487408&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R487408&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<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>

# 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>hvpap:</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinppl:</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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