

# Benzoic acid, 2,4-dihydroxy-6-methyl-, methyl ester

<b>Other names:</b>	«beta»-Resorcylic acid, 6-methyl-, methyl ester Methyl o-orsellinate Methyl orsellinate Methyl 2,4-dihydroxy-6-methylbenzoate Orsellinic acid monomethyl ester
<b>Inchi:</b>	InChI=1S/C9H10O4/c1-5-3-6(10)4-7(11)8(5)9(12)13-2/h3-4,10-11H,1-2H3
<b>InchiKey:</b>	NCCWCZLEACWJIN-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O4
<b>SMILES:</b>	<chem>COC(=O)c1c(C)cc(O)cc1O</chem>
<b>Mol. weight [g/mol]:</b>	182.17
<b>CAS:</b>	3187-58-4

## Physical Properties

Property code	Value	Unit	Source
gf	-415.48	kJ/mol	Joback Method
hf	-603.45	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	73.75	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	1.193		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
rinpol	1684.60		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	674.51	K	Joback Method
tc	912.02	K	Joback Method
tf	525.73	K	Joback Method
vc	0.388	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.94	J/molxK	674.51	Joback Method

cpg	354.52	J/mol×K	714.10	Joback Method
cpg	363.55	J/mol×K	753.68	Joback Method
cpg	372.15	J/mol×K	793.27	Joback Method
cpg	380.44	J/mol×K	832.85	Joback Method
cpg	388.51	J/mol×K	872.44	Joback Method
cpg	396.49	J/mol×K	912.02	Joback Method
dvisc	0.0000400	Paxs	525.73	Joback Method
dvisc	0.0000228	Paxs	550.53	Joback Method
dvisc	0.0000137	Paxs	575.32	Joback Method
dvisc	0.0000086	Paxs	600.12	Joback Method
dvisc	0.0000056	Paxs	624.92	Joback Method
dvisc	0.0000037	Paxs	649.71	Joback Method
dvisc	0.0000026	Paxs	674.51	Joback Method

## Sources

<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=C3187584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3187584&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hvap:</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>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

**vc:** Critical Volume

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