Benzoic acid, 2,4-dihydroxy-3,6-dimethyl-, methyl ester

Other names:	2,4-Dihydroxy-3,6-dimethylbenzoic acid, methyl ester
	Atraric acid
	Methyl 2,4-dihydroxy-3,6-dimethylbenzoate
	Methyl 3,6-dimethyl-«beta»-resorcylate
	Methyl 3,6-dimethyl-Â«betaÂ»-resorcylate
	Methyl 3,6-dimethylresorcylate
	Methyl «beta»-orcinolcarboxylate
	Methyl Â«betaÂ»-orcinolcarboxylate
	Veramoss
	«beta»-Resorcylic acid, 3,6-dimethyl-, methyl ester
	Â«betaÂ»-Resorcylic acid, 3,6-dimethyl-, methyl ester
Inchi:	InChI=1S/C10H12O4/c1-5-4-7(11)6(2)9(12)8(5)10(13)14-3/h4,11-12H,1-3H3
InchiKey:	UUQHKWMIDYRWHH-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COC(=O)c1c(C)cc(O)c(C)c1O
Mol. weight [g/mol]:	196.20
CAS:	4707-47-5

Physical Properties

Property code	Value	Unit	Source
gf	-416.69	kJ/mol	Joback Method
hf	-635.56	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.501		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
rinpol	1670.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1734.70		NIST Webbook
rinpol	1734.70		NIST Webbook
tb	702.37	K	Joback Method
tc	936.00	K	Joback Method

tf	419.77	K	Solubility and Thermodynamic Behavior of Veramoss in Different Pure Solvents and {Ethanol + Water} Mixtures from T = 283.15 to 333.15 K
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.81	J/mol×K	702.37	Joback Method
cpg	402.15	J/mol×K	741.31	Joback Method
cpg	411.99	J/mol×K	780.25	Joback Method
cpg	421.43	J/mol×K	819.18	Joback Method
cpg	430.57	J/mol×K	858.12	Joback Method
cpg	439.52	J/mol×K	897.06	Joback Method
cpg	448.37	J/mol×K	936.00	Joback Method
dvisc	0.0000245	Pa×s	549.52	Joback Method
dvisc	0.0000144	Pa×s	575.00	Joback Method
dvisc	0.0000089	Pa×s	600.47	Joback Method
dvisc	0.0000057	Pa×s	625.95	Joback Method
dvisc	0.0000038	Pa×s	651.42	Joback Method
dvisc	0.0000026	Pa×s	676.90	Joback Method
dvisc	0.0000018	Pa×s	702.37	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and Thermodynamic Behavior of Veramoss in Different Pure Solvents and {Ethanol + Water} Mixtures from T = 283.15 to 333.15 K:	https://www.doi.org/10.1021/acs.jced.6b00646
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4707475&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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