Methyl 2,6-dihydroxy-4-methylbenzoate

Other names:	Benzoic acid, 2,6-dihydroxy-4-methyl-, methyl ester Resorcylic acid,«gamma», 4-methyl-,methyl ester methyl 2,6-dihydroxy-p-toluate
Inchi:	InChI=1S/C9H10O4/c1-5-3-6(10)8(7(11)4-5)9(12)13-2/h3-4,10-11H,1-2H3
InchiKey:	RIJMQNGJNNAAQK-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COC(=O)c1c(O)cc(C)cc1O
Mol. weight [g/mol]:	182.17
CAS:	16846-10-9

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	1474.00		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/mol×K	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	Pa×s	525.73	Joback Method
dvisc	0.0000228	Pa×s	550.53	Joback Method
dvisc	0.0000137	Pa×s	575.32	Joback Method
dvisc	0.0000086	Pa×s	600.12	Joback Method
dvisc	0.0000056	Pa×s	624.92	Joback Method
dvisc	0.0000037	Pa×s	649.71	Joback Method
dvisc	0.0000026	Pa×s	674.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16846109&Units=SI

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

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