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]: 182.18

Physical Properties

Property code	Value	Unit	Source
hf	-661.51	kJ/mol	Cheméo Relay (1.0)
hfus	27.07	kJ/mol	Joback Method
hvap	82.94	kJ/mol	Cheméo Relay (1.0)
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
logp	1.193		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
rinpol	1474.00		NIST Webbook
tb	543.26	K	Cheméo Relay (1.0)
tc	797.36	K	Cheméo Relay (1.0)
tf	365.94	K	Cheméo Relay (1.0)

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16846109&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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