Methyl 4-hydroxy-3-methoxybenzoate

Other names:	Vanillic acid, methyl ester
	Methyl vanillate
	Methyl 3-methoxy-4-hydroxybenzoate
	Methyl 4-hydroxy-3-methoxybenzoate
	4-Hydroxy-3-methoxybenzoic acid methyl ester
	Methyl ester of 4-hydroxy-3-methoxybenzoic acid
	Vanillic acid methyl
	4-Hydroxy-3-methoxybenzoic acid methyl ester (methyl vanillate)
Inchi:	InChI=1S/C9H10O4/c1-12-8-5-6(9(11)13-2)3-4-7(8)10/h3-5,10H,1-2H3
InchiKey:	BVWTXUYLKBHMOX-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COC(=O)c1ccc(O)c(OC)c1
Mol. weight [g/mol]:	182.18

Physical Properties

Property code	Value	Unit	Source
af	0.6948		Cheméo Relay (1.0)
hf	-617.82	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
hvap	81.27	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-2.06		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1516.90		NIST Webbook
rinpol	1481.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook

ripol	2629.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2586.00		NIST Webbook
ripol	2578.00		NIST Webbook
ripol	2607.00		NIST Webbook
ripol	2603.00		NIST Webbook
ripol	2604.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2565.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2635.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2629.00		NIST Webbook
ripol	2598.00		NIST Webbook
ripol	2567.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2600.00		NIST Webbook
ripol	2585.00		NIST Webbook
ripol	2580.00		NIST Webbook
ripol	2586.00		NIST Webbook
tb	559.20	K	NIST Webbook
tc	770.18	K	Cheméo Relay (1.0)
tf	393.61	K	Cheméo Relay (1.0)
vc	0.484	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/mol×K	616.31	Joback Method
cpg	336.25	J/mol×K	653.92	Joback Method
cpg	346.47	J/mol×K	691.52	Joback Method
cpg	356.09	J/mol×K	729.13	Joback Method
cpg	365.12	J/mol×K	766.73	Joback Method
cpg	373.62	J/mol×K	804.34	Joback Method
cpg	381.62	J/mol×K	841.94	Joback Method
dvisc	0.0004335	Pa×s	436.24	Joback Method
dvisc	0.0002352	Pa×s	466.25	Joback Method

dvisc	0.0001374	Pa×s	496.26	Joback Method
dvisc	0.0000854	Pa×s	526.28	Joback Method
dvisc	0.0000558	Pa×s	556.29	Joback Method
dvisc	0.0000381	Pa×s	586.30	Joback Method
dvisc	0.0000270	Pa×s	616.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3943746&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume