BENZOIC ACID, 2-HYDROXY-4-METHOXY-6-METHYL-, METHYL ESTER

Other names: Methyl 2-hydroxy-4-methoxy-6-methylbenzoate
Methyl everninate

Inchi: InChI=1S/C10H12O4/c1-6-4-7(13-2)5-8(11)9(6)10(12)14-3/h4-5,11H,1-3H3

InchiKey: PFVPJOAAHSOENR-UHFFFAOYSA-N

Formula: C10H12O4

SMILES: COC(=O)c1c(C)cc(OC)cc1O

Mol. weight [g/mol]: 196.20

Physical Properties

Property code	Value	Unit	Source
hf	-637.95	kJ/mol	Cheméo Relay (1.0)
hfus	24.68	kJ/mol	Joback Method
ie	7.96	eV	Cheméo Relay (1.0)
log10ws	-3.05		Cheméo Relay (1.0)
logp	1.496		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
tb	548.23	K	Cheméo Relay (1.0)
tf	343.41	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.54	J/mol×K	644.17	Joback Method
cpg	383.08	J/mol×K	681.23	Joback Method
cpg	393.99	J/mol×K	718.30	Joback Method
cpg	404.28	J/mol×K	755.36	Joback Method
cpg	413.99	J/mol×K	792.43	Joback Method
cpg	423.15	J/mol×K	829.49	Joback Method
cpg	431.80	J/mol×K	866.56	Joback Method
dvisc	0.0002824	Pa×s	460.03	Joback Method
dvisc	0.0001598	Pa×s	490.72	Joback Method
dvisc	0.0000967	Pa×s	521.41	Joback Method
dvisc	0.0000619	Pa×s	552.10	Joback Method
dvisc	0.0000415	Pa×s	582.79	Joback Method

dvisc	0.0000290	Pa×s	613.48	Joback Method
dvisc	0.0000209	Pa×s	644.17	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C520434&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point