Benzoic acid, 2-hydroxy-4-methoxy-6-methyl-, methyl ester

Other names: Methyl everninate
Methyl 2-hydroxy-4-methoxy-6-methylbenzoate
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
CAS: 520-43-4

Physical Properties

Property code	Value	Unit	Source
gf	-367.07	kJ/mol	Joback Method
hf	-590.47	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.496		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1580.00		NIST Webbook
tb	644.17	K	Joback Method
tc	866.56	K	Joback Method
tf	460.03	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.54	J/mol×K	644.17	Joback Method
cpg	423.15	J/mol×K	829.49	Joback Method

cpg	413.99	J/mol×K	792.43	Joback Method
cpg	404.28	J/mol×K	755.36	Joback Method
cpg	393.99	J/mol×K	718.30	Joback Method
cpg	383.08	J/mol×K	681.23	Joback Method
cpg	431.80	J/mol×K	866.56	Joback Method
dvisc	0.0000209	Pa×s	644.17	Joback Method
dvisc	0.0000290	Pa×s	613.48	Joback Method
dvisc	0.0000415	Pa×s	582.79	Joback Method
dvisc	0.0000619	Pa×s	552.10	Joback Method
dvisc	0.0000967	Pa×s	521.41	Joback Method
dvisc	0.0001598	Pa×s	490.72	Joback Method
dvisc	0.0002824	Pa×s	460.03	Joback Method

Sources

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

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