

Benzoic acid, 4-hydroxy-2-methoxy-3,6-dimethyl-, methyl

Inchi:	InChI=1S/C11H14O4/c1-6-5-8(12)7(2)10(14-3)9(6)11(13)15-4/h5,12H,1-4H3
ester InchiKey:	LPHVUYDIEIQKTA-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COC(=O)c1c(C)cc(O)c(C)c1OC
Mol. weight [g/mol]:	210.23
CAS:	34874-75-4

Physical Properties

Property code	Value	Unit	Source
gf	-368.28	kJ/mol	Joback Method
hf	-622.58	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	68.92	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	1.804		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	672.03	K	Joback Method
tc	891.40	K	Joback Method
tf	483.82	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.30	J/molxK	672.03	Joback Method
cpg	431.47	J/molxK	708.59	Joback Method
cpg	443.00	J/molxK	745.15	Joback Method
cpg	453.91	J/molxK	781.71	Joback Method
cpg	464.23	J/molxK	818.28	Joback Method
cpg	473.99	J/molxK	854.84	Joback Method
cpg	483.20	J/molxK	891.40	Joback Method
dvisc	0.0001903	Paxs	483.82	Joback Method
dvisc	0.0001118	Paxs	515.19	Joback Method

dvisc	0.0000698	Paxs	546.56	Joback Method
dvisc	0.0000458	Paxs	577.92	Joback Method
dvisc	0.0000315	Paxs	609.29	Joback Method
dvisc	0.0000224	Paxs	640.66	Joback Method
dvisc	0.0000165	Paxs	672.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C34874754&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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