Benzoic acid, 4-hydroxy-3-methoxy-, ethyl ester

Other names: Vanillic acid, ethyl ester
Ethyl vanillate
4-Hydroxy-3-methoxybenzoic acid ethyl ester
Ethyl 4-hydroxy-3-methoxybenzoate
m-Anisic acid, 4-hydroxy-, ethyl ester
3-Methoxy-4-hydroxybenzoic acid, ethyl ester

Inchi: InChI=1S/C10H12O4/c1-3-14-10(12)7-4-5-8(11)9(6-7)13-2/h4-6,11H,3H2,1-2H3

InchiKey: MWAYRGBWOVHDDZ-UHFFFAOYSA-N

Formula: C10H12O4

SMILES: CCOC(=O)c1ccc(O)c(OC)c1

Mol. weight [g/mol]: 196.20

CAS: 617-05-0

Physical Properties

Property code	Value	Unit	Source
gf	-357.44	kJ/mol	Joback Method
hf	-579.00	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.577		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1574.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1589.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1589.00		NIST Webbook
ripol	2653.00		NIST Webbook
ripol	2676.00		NIST Webbook

ripol	2612.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2661.00		NIST Webbook
ripol	2614.00		NIST Webbook
ripol	2654.00		NIST Webbook
ripol	2612.00		NIST Webbook
ripol	2654.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2623.00		NIST Webbook
ripol	2616.00		NIST Webbook
ripol	2668.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2653.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2676.00		NIST Webbook
ripol	2615.00		NIST Webbook
ripol	2654.00		NIST Webbook
ripol	2665.00		NIST Webbook
tb	639.19	K	Joback Method
tc	860.68	K	Joback Method
tf	447.51	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.77	J/mol×K	639.19	Joback Method
cpg	384.49	J/mol×K	676.10	Joback Method
cpg	395.53	J/mol×K	713.02	Joback Method
cpg	405.91	J/mol×K	749.93	Joback Method
cpg	415.69	J/mol×K	786.85	Joback Method
cpg	424.90	J/mol×K	823.76	Joback Method
cpg	433.57	J/mol×K	860.68	Joback Method
dvisc	0.0003718	Pa×s	447.51	Joback Method
dvisc	0.0001978	Pa×s	479.46	Joback Method
dvisc	0.0001139	Pa×s	511.40	Joback Method
dvisc	0.0000700	Pa×s	543.35	Joback Method
dvisc	0.0000454	Pa×s	575.30	Joback Method
dvisc	0.0000308	Pa×s	607.24	Joback Method
dvisc	0.0000217	Pa×s	639.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C617050&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
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