Benzoic acid, 3-methoxy-4-methyl-

Other names:	3-Methoxy-4-methylbenzoic acid
	3-Methoxy-p-toluic acid
	4-methyl-m-anisic acid
Inchi:	InChI=1S/C9H10O3/c1-6-3-4-7(9(10)11)5-8(6)12-2/h3-5H,1-2H3,(H,10,11)
InchiKey:	CEAVPXDEPGAVDA-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cc(C(=O)O)ccc1C
Mol. weight [g/mol]:	166.17
CAS:	7151-68-0

Physical Properties

Property code	Value	Unit	Source
gf	-252.69	kJ/mol	Joback Method
hf	-412.53	kJ/mol	Joback Method
hfus	19.20	kJ/mol	Joback Method
hvap	65.06	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.702		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	610.43	K	Joback Method
tc	813.59	K	Joback Method
tf	375.63	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.85	J/mol×K	610.43	Joback Method
cpg	311.80	J/mol×K	644.29	Joback Method
cpg	321.22	J/mol×K	678.15	Joback Method
cpg	330.11	J/mol×K	712.01	Joback Method
cpg	338.49	J/mol×K	745.87	Joback Method
cpg	346.35	J/mol×K	779.73	Joback Method

cpg	353.71	J/mol×K	813.59	Joback Method
dvisc	0.0019634	Pa×s	375.63	Joback Method
dvisc	0.0008840	Pa×s	414.76	Joback Method
dvisc	0.0004568	Pa×s	453.90	Joback Method
dvisc	0.0002621	Pa×s	493.03	Joback Method
dvisc	0.0001632	Pa×s	532.16	Joback Method
dvisc	0.0001084	Pa×s	571.30	Joback Method
dvisc	0.0000759	Pa×s	610.43	Joback Method

Sources

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=C7151680&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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