Benzoic acid, 3-methoxy-, methyl ester

Other names:	m-Anisic acid, methyl ester
	m-Methoxybenzoic acid methyl ester
	Methyl m-anisate
	Methyl m-methoxybenzoate
	Methyl 3-methoxybenzoate
	3-Methoxybenoic acid methyl ester
	3-Methoxybenzoic acid methyl ester
	Methyl ester of m-Methoxybenzoic acid
	3-CH3O-C6H4-COOCH3
	NSC 100922
Inchi:	InChI=1S/C9H10O3/c1-11-8-5-3-4-7(6-8)9(10)12-2/h3-6H,1-2H3
InchiKey:	DUKYPQBGYRJVAN-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	166.17
CAS:	5368-81-0

Physical Properties

Property code	Value	Unit	Source
affp	856.70	kJ/mol	NIST Webbook
basg	825.80	kJ/mol	NIST Webbook
gf	-211.24	kJ/mol	Joback Method
hf	-381.05	kJ/mol	Joback Method
hfus	16.69	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.482		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1352.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1358.90		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1358.90		NIST Webbook
rinpol	1331.00		NIST Webbook

tb	535.69	K	Joback Method
tc	750.72	K	Joback Method
tf	324.52	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.97	J/mol×K	535.69	Joback Method
cpg	291.01	J/mol×K	571.53	Joback Method
cpg	302.48	J/mol×K	607.37	Joback Method
cpg	313.35	J/mol×K	643.20	Joback Method
cpg	323.62	J/mol×K	679.04	Joback Method
cpg	333.30	J/mol×K	714.88	Joback Method
cpg	342.37	J/mol×K	750.72	Joback Method
dvisc	0.0013483	Pa×s	324.52	Joback Method
dvisc	0.0008247	Pa×s	359.72	Joback Method
dvisc	0.0005507	Pa×s	394.91	Joback Method
dvisc	0.0003928	Pa×s	430.11	Joback Method
dvisc	0.0002949	Pa×s	465.30	Joback Method
dvisc	0.0002305	Pa×s	500.50	Joback Method
dvisc	0.0001861	Pa×s	535.69	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5368810&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

affp: Proton affinity

basg: Gas basicity

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