Benzoic acid, 3-methoxy-

Other names:	3-methoxybenzoic acid
	m-Methoxybenzoic acid
	m-anisic acid
Inchi:	InChI=1S/C8H8O3/c1-11-7-4-2-3-6(5-7)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	XHQZJYCNDZAGLW-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1cccc(C(=O)O)c1
Mol. weight [g/mol]:	152.15
CAS:	586-38-9

Physical Properties

Property code	Value	Unit	Source
chs	-3737.91 ± 0.60	kJ/mol	NIST Webbook
gf	-251.48	kJ/mol	Joback Method
hf	-446.10 ± 0.80	kJ/mol	NIST Webbook
hfs	-553.50 ± 1.20	kJ/mol	NIST Webbook
hfus	21.90	kJ/mol	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
hsub	107.50 ± 0.40	kJ/mol	NIST Webbook
hsub	107.40	kJ/mol	NIST Webbook
hsub	114.70 ± 0.80	kJ/mol	NIST Webbook
hvap	95.00	kJ/mol	NIST Webbook
ie	9.10 ± 0.20	eV	NIST Webbook
log10ws	-1.65		Crippen Method
logp	1.393		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	582.57	K	Joback Method
tc	787.82	K	Joback Method
tf	351.84	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.56	J/mol×K	753.62	Joback Method
cpg	305.30	J/mol×K	787.82	Joback Method
cpg	257.47	J/mol×K	582.57	Joback Method
cpg	266.70	J/mol×K	616.78	Joback Method
cpg	275.42	J/mol×K	650.99	Joback Method
cpg	283.63	J/mol×K	685.20	Joback Method
cpg	291.34	J/mol×K	719.41	Joback Method
dvisc	0.0000920	Pa×s	582.57	Joback Method
dvisc	0.0001345	Pa×s	544.12	Joback Method
dvisc	0.0031310	Pa×s	351.84	Joback Method
dvisc	0.0013019	Pa×s	390.30	Joback Method
dvisc	0.0006336	Pa×s	428.75	Joback Method
dvisc	0.0003472	Pa×s	467.20	Joback Method
dvisc	0.0002085	Pa×s	505.66	Joback Method
hfust	24.90	kJ/mol	378.70	NIST Webbook
hsubt	107.40 ± 0.40	kJ/mol	318.12	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	444.20	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C586389&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods: https://www.doi.org/10.1016/j.tca.2015.03.026

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume