Benzoic acid, 4-methoxy-

Other names:	4-Anisic acid
	4-Methoxybenzoic acid
	Anisic acid, para
	Draconic acid
	Kyselina 4-methoxybenzoova
	p-Anisic acid
	p-Methoxybenzoic acid
Inchi:	InChI=1S/C8H8O3/c1-11-7-4-2-6(3-5-7)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	ZEYHEAKUIGZSGI-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	152.15
CAS:	100-09-4

Physical Properties

Property code	Value	Unit	Source
chs	-3729.71 ± 0.75	kJ/mol	NIST Webbook
gf	-251.48	kJ/mol	Joback Method
hf	-451.90 ± 1.40	kJ/mol	NIST Webbook
hfs	-561.70 ± 1.30	kJ/mol	NIST Webbook
hfus	28.97	kJ/mol	Thermodynamic Study of 4-n-Alkyloxybenzoic Acids
hsub	111.60 ± 0.60	kJ/mol	NIST Webbook
hsub	109.80 ± 0.60	kJ/mol	NIST Webbook
hsub	109.80	kJ/mol	NIST Webbook
hvap	92.00	kJ/mol	NIST Webbook
ie	9.00 ± 0.20	eV	NIST Webbook
log10ws	-2.46		Aqueous Solubility Prediction Method
logp	1.393		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	1453.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1441.00		NIST Webbook

sg	413.00	J/mol×K	NIST Webbook
tb	582.57	K	Joback Method
tc	787.82	K	Joback Method
tf	456.75 ± 0.20	K	NIST Webbook
tf	457.57	K	Aqueous Solubility Prediction Method
tf	457.00 ± 1.00	K	NIST Webbook
tf	457.80 ± 0.50	K	NIST Webbook
tf	456.15 ± 1.00	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.30	J/mol×K	787.82	Joback Method
cpg	298.56	J/mol×K	753.62	Joback Method
cpg	291.34	J/mol×K	719.41	Joback Method
cpg	283.63	J/mol×K	685.20	Joback Method
cpg	275.42	J/mol×K	650.99	Joback Method
cpg	266.70	J/mol×K	616.78	Joback Method
cpg	257.47	J/mol×K	582.57	Joback Method
cps	205.00	J/mol×K	323.00	NIST Webbook
dvisc	0.0006336	Pa×s	428.75	Joback Method
dvisc	0.0000920	Pa×s	582.57	Joback Method
dvisc	0.0003472	Pa×s	467.20	Joback Method
dvisc	0.0002085	Pa×s	505.66	Joback Method
dvisc	0.0031310	Pa×s	351.84	Joback Method
dvisc	0.0013019	Pa×s	390.30	Joback Method
dvisc	0.0001345	Pa×s	544.12	Joback Method
hfust	28.33	kJ/mol	456.70	NIST Webbook
hfust	29.90	kJ/mol	455.60	NIST Webbook
hfust	28.40	kJ/mol	457.80	NIST Webbook
hsubt	109.80 ± 0.60	kJ/mol	334.61	NIST Webbook
psub	0.02	kPa	394.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods

psub	0.03	kPa	397.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.03	kPa	400.30	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.04	kPa	403.40	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.05	kPa	406.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.02	kPa	391.10	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.01	kPa	388.30	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	8.50e-03	kPa	384.50	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods

psub	3.53e-03	kPa	374.90	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	1.90e-03	kPa	368.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	1.17e-03	kPa	363.30	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	7.53e-03	kPa	383.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2015.03.026
Thermodynamic Study of 4-n-Alkyloxybenzoic Acids:	https://www.doi.org/10.1021/je900776y
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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