

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	109.80	kJ/mol	NIST Webbook
hsub	109.80 ± 0.60	kJ/mol	NIST Webbook
hsub	111.60 ± 0.60	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	1441.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1453.00		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	457.80 ± 0.50	K	NIST Webbook
tf	457.00 ± 1.00	K	NIST Webbook
tf	457.57	K	Aqueous Solubility Prediction Method
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	291.34	J/mol×K	719.41	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
cpg	298.56	J/mol×K	753.62	Joback Method
cpg	305.30	J/mol×K	787.82	Joback Method
cpg	283.63	J/mol×K	685.20	Joback Method
cps	205.00	J/mol×K	323.00	NIST Webbook
dvisc	0.0006336	Paxs	428.75	Joback Method
dvisc	0.0003472	Paxs	467.20	Joback Method
dvisc	0.0031310	Paxs	351.84	Joback Method
dvisc	0.0002085	Paxs	505.66	Joback Method
dvisc	0.0001345	Paxs	544.12	Joback Method
dvisc	0.0000920	Paxs	582.57	Joback Method
dvisc	0.0013019	Paxs	390.30	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	0.01	kPa	388.30	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	0.03	kPa	397.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
psub	0.02	kPa	394.20	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	0.04	kPa	403.40	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	7.53e-03	kPa	383.20	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	0.05	kPa	406.20	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods

Sources

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 Alkoxobenzoic Acids: <https://www.doi.org/10.1021/je900776y>

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

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>

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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