

Benzoic acid, 2-methoxy-

Other names:	2-Anisic acid 2-Methoxybenzoic acid Kyselina 2-methoxybenzoova NSC 3778 O-Methylsalicylic acid Salicylic acid methyl ether o-Anisic acid o-Methoxybenzoic acid
Inchi:	InChI=1S/C8H8O3/c1-11-7-5-3-2-4-6(7)8(9)10/h2-5H,1H3,(H,9,10)
InchiKey:	ILUJQPXNXACGAN-UHFFFAOYSA-N
Formula:	C8H8O3
SMILES:	COc1ccccc1C(=O)O
Mol. weight [g/mol]:	152.15
CAS:	579-75-9

Physical Properties

Property code	Value	Unit	Source
chs	-3752.88 ± 0.64	kJ/mol	NIST Webbook
gf	-251.48	kJ/mol	Joback Method
hf	-433.80 ± 1.20	kJ/mol	NIST Webbook
hfs	-538.50 ± 1.20	kJ/mol	NIST Webbook
hfus	23.90	kJ/mol	Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods
hsub	104.70 ± 0.30	kJ/mol	NIST Webbook
hsub	110.70 ± 0.80	kJ/mol	NIST Webbook
hsub	90.90 ± 0.40	kJ/mol	NIST Webbook
hsub	104.70	kJ/mol	NIST Webbook
hvap	91.80	kJ/mol	NIST Webbook
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	1.393		Crippen Method
mvol	113.130	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	1490.00		NIST Webbook
tb	582.57	K	Joback Method

tc	787.82	K	Joback Method
tf	373.65	K	Aqueous Solubility Prediction Method
tf	370.00 ± 6.00	K	NIST Webbook
tf	374.05 ± 0.50	K	NIST Webbook
tf	374.45	K	KDB
tf	374.00 ± 3.00	K	NIST Webbook
vc	0.418	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.30	J/mol×K	787.82	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
cpg	298.56	J/mol×K	753.62	Joback Method
cpg	257.47	J/mol×K	582.57	Joback Method
dvisc	0.0001345	Paxs	544.12	Joback Method
dvisc	0.0002085	Paxs	505.66	Joback Method
dvisc	0.0003472	Paxs	467.20	Joback Method
dvisc	0.0006336	Paxs	428.75	Joback Method
dvisc	0.0013019	Paxs	390.30	Joback Method
dvisc	0.0000920	Paxs	582.57	Joback Method
dvisc	0.0031310	Paxs	351.84	Joback Method
hfust	24.00	kJ/mol	374.60	NIST Webbook
hsubt	90.90	kJ/mol	360.50	NIST Webbook
hsubt	101.20	kJ/mol	335.50	NIST Webbook
hsubt	104.70 ± 0.30	kJ/mol	319.34	NIST Webbook
hsubt	90.80 ± 0.40	kJ/mol	360.50	NIST Webbook
psub	2.21e-03	kPa	350.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	6.80e-03	kPa	361.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study

psub	8.13e-03	kPa	363.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.01	kPa	366.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.01	kPa	367.90	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	0.02	kPa	371.50	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	9.80e-04	kPa	342.40	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	5.36e-03	kPa	358.90	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	4.19e-03	kPa	356.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	3.47e-03	kPa	354.30	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	1.52e-03	kPa	346.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study

psub	1.81e-03	kPa	348.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study
psub	2.72e-03	kPa	352.20	Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	-1.20317e+02
Coeff. B	-6.18426e+03
Coeff. C	2.28341e+01
Coeff. D	-1.51976e-05
Temperature range (K), min.	319.15
Temperature range (K), max.	335.15

Sources

KDB Vapor Pressure Data: <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=958>

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study: <https://www.doi.org/10.1016/j.tca.2015.07.011>

KDB: <https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=958>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C579759&Units=SI>

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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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