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	90.90 ± 0.40	kJ/mol	NIST Webbook
hsub	104.70 ± 0.30	kJ/mol	NIST Webbook
hsub	104.70	kJ/mol	NIST Webbook
hsub	110.70 ± 0.80	kJ/mol	NIST Webbook
hvap	91.80	kJ/mol	NIST Webbook
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	1.393		Crippen Method
mcvol	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	374.45	K	KDB
tf	374.05 ± 0.50	K	NIST Webbook
tf	370.00 ± 6.00	K	NIST Webbook
tf	374.00 ± 3.00	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	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	0.0031310	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
dvisc	0.0001345	Pa×s	544.12	Joback Method
dvisc	0.0000920	Pa×s	582.57	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	0.01	kPa	366.20	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	2.72e-03	kPa	352.20	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	2.21e-03	kPa	350.30	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	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	6.80e-03	kPa	361.40	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	8.13e-03	kPa	363.20	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*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

Thermodynamic properties of isomeric iso-butoxybenzoic acids: Experimental and theoretical study:	https://www.doi.org/10.1016/j.tca.2015.07.011
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=958
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=958
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Benzoic acid derivatives: Evaluation of thermochemical properties with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2015.03.026
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C579759&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume