Benzaldehyde, 4-methoxy-

Other names:	4-Anisaldehyde
	4-Methoxybenzaldehyde
	Anisal
	Anisaldehyde
	Anisaldehyde (para)
	Anisic aldehyde
	Aubepine
	Crategine
	Methoxybenzaldehyde
	NSC 5590
	Obepin
	p-Anisaldehyde
	p-Anisic aldehyde
	p-Formylanisole
	p-Methoxybenzaldehyde
	para-Anisaldehyde
Inchi:	InChI=1S/C8H8O2/c1-10-8-4-2-7(6-9)3-5-8/h2-6H,1H3
InchiKey:	ZRSNZINYAWTAHE-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	COc1ccc(C=O)cc1
Mol. weight [g/mol]:	136.15
CAS:	123-11-5

Physical Properties

Property code	Value	Unit	Source
affp	881.10	kJ/mol	NIST Webbook
basg	849.30	kJ/mol	NIST Webbook
chl	-4047.00	kJ/mol	NIST Webbook
chl	-4024.20 ± 7.50	kJ/mol	NIST Webbook
gf	-85.26	kJ/mol	Joback Method
hf	-201.19	kJ/mol	Joback Method
hfl	-247.00	kJ/mol	NIST Webbook
hfus	13.60	kJ/mol	Joback Method
hvap	60.40	kJ/mol	NIST Webbook
ie	8.43	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	8.60 ± 0.03	eV	NIST Webbook

ie	8.87	eV	NIST Webbook
log10ws	-1.49		Estimated Solubility Method
log10ws	-1.49		Aqueous Solubility Prediction Method
logp	1.508		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1262.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1238.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1219.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1215.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1250.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1207.00		NIST Webbook
rinpol	1206.00		NIST Webbook

rinpol	1206.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1261.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1242.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1250.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1220.40	NIST Webbook
rinpol	1230.60	NIST Webbook
rinpol	1239.60	NIST Webbook
rinpol	1231.50	NIST Webbook
rinpol	1262.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1219.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1235.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1251.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1252.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1229.00	NIST Webbook

rinpol	1207.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1238.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1249.00	NIST Webbook
rinpol	1247.00	NIST Webbook
rinpol	1239.00	NIST Webbook
rinpol	1263.00	NIST Webbook
rinpol	1248.00	NIST Webbook
ripol	2000.00	NIST Webbook
ripol	2014.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	2011.00	NIST Webbook
ripol	2006.80	NIST Webbook
ripol	2035.00	NIST Webbook
ripol	1998.00	NIST Webbook
ripol	2045.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	2048.00	NIST Webbook
ripol	2058.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	2014.00	NIST Webbook
ripol	1988.00	NIST Webbook
ripol	2030.00	NIST Webbook
ripol	2053.00	NIST Webbook
ripol	1998.00	NIST Webbook
ripol	2048.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	2011.00	NIST Webbook
ripol	1986.00	NIST Webbook
ripol	2058.00	NIST Webbook
ripol	1980.00	NIST Webbook
ripol	2052.00	NIST Webbook
ripol	2019.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	2040.00	NIST Webbook
ripol	2009.00	NIST Webbook
ripol	2009.00	NIST Webbook
ripol	2015.00	NIST Webbook
ripol	1966.00	NIST Webbook

ripol	2038.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2003.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2007.30		NIST Webbook
ripol	2006.80		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	2027.00		NIST Webbook
ripol	2016.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	1990.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2055.00		NIST Webbook
tb	521.20	K	NIST Webbook
tb	521.00	K	NIST Webbook
tb	521.15 ± 0.50	K	NIST Webbook
tb	520.15 ± 3.00	K	NIST Webbook
tb	521.15 ± 2.00	K	NIST Webbook
tc	700.43	K	Joback Method
tf	273.12 ± 0.40	K	NIST Webbook
tf	273.40	K	Aqueous Solubility Prediction Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.34	J/mol×K	592.80	Joback Method
cpg	255.42	J/mol×K	628.68	Joback Method
cpg	263.97	J/mol×K	664.55	Joback Method
cpg	215.85	J/mol×K	485.18	Joback Method
cpg	226.56	J/mol×K	521.05	Joback Method
cpg	236.72	J/mol×K	556.93	Joback Method
cpg	272.00	J/mol×K	700.43	Joback Method

dvisc	0.0037060	Pa×s	298.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0028300	Pa×s	308.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
dvisc	0.0022320	Pa×s	318.15	Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K
hvapt	58.40	kJ/mol	434.50	NIST Webbook
hvapt	57.10	kJ/mol	433.50	NIST Webbook
srf	0.09	N/m	323.15	Thermophysical Properties of para-Anisaldehyde (1) + Chlorobenzene (2) at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa
srf	0.10	N/m	313.15	Thermophysical Properties of para-Anisaldehyde (1) + Chlorobenzene (2) at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa
srf	0.10	N/m	303.15	Thermophysical Properties of para-Anisaldehyde (1) + Chlorobenzene (2) at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59651e+01
Coeff. B	-5.38153e+03
Coeff. C	-4.68710e+01
Temperature range (K), min.	390.14
Temperature range (K), max.	552.01

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123115&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess parameters of binary mixtures of anisaldehyde with o-cresol, m-cresol and p-cresol at T = (303.15, 308.15, 313.15, and 318.15) K:	https://www.doi.org/10.1016/j.jct.2011.05.018
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Density and Viscosity of Acrylonitrile + Cinnamaldehyde, + Anisaldehyde, and + Benzaldehyde at (298.15, 308.15, and 318.15) K:	https://www.doi.org/10.1021/je7006742
Thermophysical Properties of para-Anisaldehyde (1) + Chlorobenzene (2) at Temperatures of (303.15, 313.15, and 323.15) K and a Pressure of 0.1 MPa:	https://www.doi.org/10.1021/je700714m

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid 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
hfl:	Liquid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume