Benzaldehyde, 3-methoxy-

Other names:	m-Anisaldehyde
	m-Methoxybenzaldehyde
	3-Anisaldehyde
	3-Methoxybenzaldehyde
	Metamethoxybenzaldehyde
Inchi:	InChI=1S/C8H8O2/c1-10-8-4-2-3-7(5-8)6-9/h2-6H,1H3
InchiKey:	WMPDAIZRQDCGFH-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	COc1cccc(C=O)c1
Mol. weight [g/mol]:	136.15
CAS:	591-31-1

Physical Properties

Property code	Value	Unit	Source
affp	844.10	kJ/mol	NIST Webbook
basg	812.20	kJ/mol	NIST Webbook
chl	-4015.40 ± 7.50	kJ/mol	NIST Webbook
ea	0.43 ± 0.04	eV	NIST Webbook
gf	-85.26	kJ/mol	Joback Method
hf	-201.19	kJ/mol	Joback Method
hfus	13.60	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.508		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1194.00		NIST Webbook
rinpol	1194.00		NIST Webbook
rinpol	1178.60		NIST Webbook
rinpol	1176.00		NIST Webbook
rinpol	1196.30		NIST Webbook
rinpol	1187.80		NIST Webbook
rinpol	1178.60		NIST Webbook
tb	503.00	K	NIST Webbook
tc	700.43	K	Joback Method
tf	283.09	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	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	272.00	J/mol×K	700.43	Joback Method
dvisc	0.0018659	Pa×s	283.09	Joback Method
dvisc	0.0011193	Pa×s	316.77	Joback Method
dvisc	0.0007408	Pa×s	350.45	Joback Method
dvisc	0.0005270	Pa×s	384.13	Joback Method
dvisc	0.0003961	Pa×s	417.82	Joback Method
dvisc	0.0003107	Pa×s	451.50	Joback Method
dvisc	0.0002520	Pa×s	485.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	6.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591311&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume