

Benzaldehyde, 2-methoxy-

Other names:	2-anisaldehyde 2-methoxybenzaldehyde 2-methoxybenzenecarboxaldehyde 6-Methoxybenzaldehyde Benzaldehyde, o-methoxy- o-Methoxybenzaldehyde o-anisaldehyde salicylaldehyde methyl ether
Inchi:	InChI=1S/C8H8O2/c1-10-8-5-3-2-4-7(8)6-9/h2-6H,1H3
InchiKey:	PKZJLOCLABXVMC-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	COc1ccccc1C=O
Mol. weight [g/mol]:	136.15
CAS:	135-02-4

Physical Properties

Property code	Value	Unit	Source
chs	-4025.00 ± 7.50	kJ/mol	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	1242.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1222.50		NIST Webbook
rinpol	1227.90		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1222.50		NIST Webbook
ripol	1941.00		NIST Webbook
ripol	1941.00		NIST Webbook
tb	516.70	K	NIST Webbook
tb	516.00	K	NIST Webbook
tb	511.20	K	NIST Webbook

tb	516.15 ± 1.50	K	NIST Webbook
tc	700.43	K	Joback Method
tf	308.15 ± 0.50	K	NIST Webbook
vc	0.410	m ³ /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

Sources

Construction of solid liquid phase diagrams in ternary systems by the law of regularity:

McGowan Method:

NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.tca.2006.02.017>

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C135024&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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