

3-METHYL-PARA-ANISALDEHYDE

Other names:	3-Methyl-para-anisaldehyde 3-methyl-4-anisaldehyde Benzaldehyde, 4-methoxy-3-methyl-
Inchi:	InChI=1S/C9H10O2/c1-7-5-8(6-10)3-4-9(7)11-2/h3-6H,1-2H3
InchiKey:	MYLBIQHZWFWSMH-UHFFFAOYSA-N
Formula:	C9H10O2
SMILES:	COc1ccc(C=O)cc1C
Mol. weight [g/mol]:	150.18

Physical Properties

Property code	Value	Unit	Source
hfus	15.81	kJ/mol	Joback Method
hvap	65.72	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-1.79		Cheméo Relay (1.0)
logp	1.816		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
tb	520.81	K	Cheméo Relay (1.0)
tc	741.14	K	Cheméo Relay (1.0)
tf	307.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.40	J/mol×K	513.04	Joback Method
cpg	318.32	J/mol×K	726.15	Joback Method
cpg	309.53	J/mol×K	690.64	Joback Method
cpg	300.20	J/mol×K	655.12	Joback Method
cpg	290.33	J/mol×K	619.60	Joback Method
cpg	279.91	J/mol×K	584.08	Joback Method
cpg	268.93	J/mol×K	548.56	Joback Method
dvisc	0.0004649	Pa×s	409.96	Joback Method
dvisc	0.0002337	Pa×s	513.04	Joback Method
dvisc	0.0002844	Pa×s	478.68	Joback Method

dvisc	0.0003568	Pa×s	444.32	Joback Method
dvisc	0.0014682	Pa×s	306.88	Joback Method
dvisc	0.0006359	Pa×s	375.60	Joback Method
dvisc	0.0009264	Pa×s	341.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.70	K	0.10	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C32723674&Units=SI>

Joback Method:

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

McGowan Method:

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

Crippen Method:

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

Crippen Method:

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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