METHYL 2-METHOXYBENZOATE

Other names:	2-Methoxybenzoic acid, methyl ester
	Benzoic acid, 2-methoxy-, methyl ester
	Benzoic acid, o-methoxy-, methyl ester
	Dimethyl derivative of Salicylic acid
	Dimethyl salicylate
	Methyl ester of o-Methoxybenzoic acid
	Methyl o-anisate
	Methyl o-methoxybenzoate
	Methylsalicylate methyl ether
	NSC 406256
	o-Anisic acid, methyl ester
	o-Methoxy methyl benzoate
	o-Methoxybenzoic acid methyl ester
Inchi:	InChI=1S/C9H10O3/c1-11-8-6-4-3-5-7(8)9(10)12-2/h3-6H,1-2H3
InchiKey:	PFYHAAAQPNMZHO-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(=O)c1ccccc1OC
Mol. weight [g/mol]:	166.18

Physical Properties

Property code	Value	Unit	Source
af	0.5440		Cheméo Relay (1.0)
hf	-422.74	kJ/mol	Cheméo Relay (1.0)
hfus	16.69	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-2.34		Cheméo Relay (1.0)
logp	1.482		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1298.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1293.00		NIST Webbook

rinpol	1295.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1351.30		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1351.30		NIST Webbook
rinpol	1336.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2049.00		NIST Webbook
tb	521.20	K	NIST Webbook
tc	721.00	K	Cheméo Relay (1.0)
tf	275.39	K	Cheméo Relay (1.0)
tt	276.42	K	Thermochemical Study of Methyl n-Methoxybenzoates: An Experimental and Computational Approach
vc	0.470	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.97	J/mol×K	535.69	Joback Method
cpg	291.01	J/mol×K	571.53	Joback Method
cpg	302.48	J/mol×K	607.37	Joback Method
cpg	313.35	J/mol×K	643.20	Joback Method
cpg	323.62	J/mol×K	679.04	Joback Method
cpg	333.30	J/mol×K	714.88	Joback Method
cpg	342.37	J/mol×K	750.72	Joback Method
dvisc	0.0013483	Pa×s	324.52	Joback Method

dvisc	0.0008247	Pa×s	359.72	Joback Method
dvisc	0.0005507	Pa×s	394.91	Joback Method
dvisc	0.0003928	Pa×s	430.11	Joback Method
dvisc	0.0002949	Pa×s	465.30	Joback Method
dvisc	0.0002305	Pa×s	500.50	Joback Method
dvisc	0.0001861	Pa×s	535.69	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.20	K	1.50	NIST Webbook

Sources

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

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

Cheméo Relay (1.0):

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

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

Thermochemical Study of Methyl n-Methoxybenzoates: An Experimental and Computational Approach: https://www.doi.org/10.1021/acs.jced.8b00978

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C606451&Units=SI

KDB: https://www.cheric.org/files/research/kdb/mol/mol1144.mol

Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume