Benzoic acid, 2-methoxy-, methyl ester

Other names:	2-Methoxybenzoic acid, methyl ester
	Benzoic acid, o-methoxy-, methyl ester
	Dimethyl derivative of Salicylic acid
	Dimethyl salicylate
	Methyl 2-methoxybenzoate
	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]:	166.17
CAS:	606-45-1

Physical Properties

Property code	Value	Unit	Source
gf	-211.24	kJ/mol	Joback Method
hf	-381.05	kJ/mol	Joback Method
hfus	16.69	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.482		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1337.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1303.00		NIST Webbook

rinpol	1303.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1341.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1351.30		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1351.30		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2049.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2032.00		NIST Webbook
ripol	2073.00		NIST Webbook
tb	521.20	K	NIST Webbook
tc	750.72	K	Joback Method
tf	324.52	K	Joback Method
tt	276.42	K	Thermochemical Study of Methyl n-Methoxybenzoates: An Experimental and Computational Approach
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.97	J/mol×K	535.69	Joback Method
cpg	333.30	J/mol×K	714.88	Joback Method
cpg	323.62	J/mol×K	679.04	Joback Method
cpg	313.35	J/mol×K	643.20	Joback Method
cpg	302.48	J/mol×K	607.37	Joback Method
cpg	291.01	J/mol×K	571.53	Joback Method
cpg	342.37	J/mol×K	750.72	Joback Method
dvisc	0.0001861	Pa×s	535.69	Joback Method

dvisc	0.0002305	Pa×s	500.50	Joback Method
dvisc	0.0002949	Pa×s	465.30	Joback Method
dvisc	0.0003928	Pa×s	430.11	Joback Method
dvisc	0.0005507	Pa×s	394.91	Joback Method
dvisc	0.0008247	Pa×s	359.72	Joback Method
dvisc	0.0013483	Pa×s	324.52	Joback Method

Pressure Dependent Properties

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

Sources

Thermochemical Study of Methyl n-Methoxybenzoates: An Experimental and Computational Approach:	https://www.doi.org/10.1021/acs.jced.8b00978
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1144.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C606451&Units=SI
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume