Benzoic acid, 4-formyl-, methyl ester

Other names:	p-Carbomethoxybenzaldehyde
	4-Carbomethoxybenzaldehyde
	4-Carboxybenzaldehyde methyl ester
	p-Formylbenzoic acid methyl ester
	4-(Methoxycarbonyl)benzaldehyde
	Methyl benzaldehyde-4-carboxylate
	Methyl p-formylbenzoate
	Methyl 4-formylbenzoate
	Methyl terephthalaldehydate
	Terephthalaldehydic acid, methyl ester
	p-Methoxycarbonylbenzaldehyde
	Methyl terephthaldehydate
	4-HC(O)-C6H4-COOCH3
	4-Formylbenzoic acid methyl ester
	NSC 28459
Inchi:	InChI=1S/C9H8O3/c1-12-9(11)8-4-2-7(6-10)3-5-8/h2-6H,1H3
InchiKey:	FEIOASZZURHTHB-UHFFFAOYSA-N
Formula:	C9H8O3
SMILES:	COC(=O)c1ccc(C=O)cc1
Mol. weight [g/mol]:	164.16
CAS:	1571-08-0

Physical Properties

Property code	Value	Unit	Source
affp	832.90	kJ/mol	NIST Webbook
basg	801.90	kJ/mol	NIST Webbook
ea	1.05 ± 0.09	eV	NIST Webbook
ea	1.16 ± 0.09	eV	NIST Webbook
gf	-205.76	kJ/mol	Joback Method
hf	-334.41	kJ/mol	Joback Method
hfus	17.79	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.286		Crippen Method
mcvol	122.920	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	538.20	K	NIST Webbook

tc	782.61	K	Joback Method
tf	344.29	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.43	J/mol×K	561.93	Joback Method
cpg	282.25	J/mol×K	598.71	Joback Method
cpg	292.43	J/mol×K	635.49	Joback Method
cpg	301.97	J/mol×K	672.27	Joback Method
cpg	310.88	J/mol×K	709.05	Joback Method
cpg	319.18	J/mol×K	745.83	Joback Method
cpg	326.87	J/mol×K	782.61	Joback Method
dvisc	0.0018131	Pa×s	344.29	Joback Method
dvisc	0.0011322	Pa×s	380.56	Joback Method
dvisc	0.0007674	Pa×s	416.84	Joback Method
dvisc	0.0005535	Pa×s	453.11	Joback Method
dvisc	0.0004191	Pa×s	489.38	Joback Method
dvisc	0.0003297	Pa×s	525.66	Joback Method
dvisc	0.0002676	Pa×s	561.93	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1571080&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume