

4-Fluorobenzoic acid, methyl ester

Other names:	4-F-C6H4-COOCH3 Benzoic acid, 4-fluoro-, methyl ester Benzoic acid, p-fluoro-, methyl ester Methyl p-fluorobenzoate p-Fluorobenzoic acid, methyl ester
Inchi:	InChI=1S/C8H7FO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,1H3
InchiKey:	MSEBQGULDWDIRW-UHFFFAOYSA-N
Formula:	C8H7FO2
SMILES:	COC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	154.14

Physical Properties

Property code	Value	Unit	Source
af	0.4544		Cheméo Relay (1.0)
affp	841.30	kJ/mol	NIST Webbook
basg	810.30	kJ/mol	NIST Webbook
hf	-499.72	kJ/mol	Cheméo Relay (1.0)
hfus	15.99	kJ/mol	Joback Method
hvap	62.89	kJ/mol	Cheméo Relay (1.0)
ie	9.38	eV	Cheméo Relay (1.0)
log10ws	-2.34		Cheméo Relay (1.0)
logp	1.612		Crippen Method
mcvol	109.030	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
rinpol	1074.00		NIST Webbook
rinpol	1062.00		NIST Webbook
tb	469.46	K	Cheméo Relay (1.0)
tc	670.80	K	Cheméo Relay (1.0)
tf	273.70	K	The influence of the halogen size in the volatility and melting of methyl p-halobenzoic esters and of their parent acids
vc	0.401	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.54	J/mol×K	489.66	Joback Method
cpg	233.02	J/mol×K	524.56	Joback Method
cpg	242.97	J/mol×K	559.46	Joback Method
cpg	252.38	J/mol×K	594.36	Joback Method
cpg	261.27	J/mol×K	629.26	Joback Method
cpg	269.64	J/mol×K	664.16	Joback Method
cpg	277.50	J/mol×K	699.06	Joback Method

Sources

Cheméo Relay (1.0, beta):

The influence of the halogen size in the volatility and melting of methyl
haloalkanoates and of their
parent acids:
Joback Method:

<https://www.doi.org/10.1016/j.jct.2012.07.027>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C403338&Units=SI>

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

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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<https://www.chemeo.com/cid/12-840-5/4-Fluorobenzoic-acid-methyl-ester.pdf>

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