

Methyl 4-fluorobenzoate

Other names:	4-F-C6H4-COOCH3 4-Fluorobenzoic acid, methyl ester 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
CAS:	403-33-8

Physical Properties

Property code	Value	Unit	Source
affp	841.30	kJ/mol	NIST Webbook
basg	810.30	kJ/mol	NIST Webbook
gf	-309.47	kJ/mol	Joback Method
hf	-424.30	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
log10ws	-2.05		Crippen Method
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	489.66	K	Joback Method
tc	699.06	K	Joback Method
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	0.417	m3/kmol	

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

The influence of the halogen size in the volatility and melting of methyl esters and of their parent acids: <https://www.doi.org/10.1016/j.jct.2012.07.027>
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C403338&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
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
mccvol: 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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