

# Benzene, 1-fluoro-4-methoxy-

<b>Other names:</b>	1-fluoro-4-methoxybenzene 4-fluoroanisole 4-fluoromethoxybenzene anisole, p-fluoro- p-Fluoromethoxybenzene p-Fluorophenyl methyl ether p-Methoxyfluorobenzene p-fluoroanisol p-fluoroanisole
<b>Inchi:</b>	InChI=1S/C7H7FO/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
<b>InchiKey:</b>	VIPWUFMFHBIKQI-UHFFFAOYSA-N
<b>Formula:</b>	C7H7FO
<b>SMILES:</b>	COc1ccc(F)cc1
<b>Mol. weight [g/mol]:</b>	126.13
<b>CAS:</b>	459-60-9

## Physical Properties

Property code	Value	Unit	Source
affp	795.00	kJ/mol	NIST Webbook
basg	767.00	kJ/mol	NIST Webbook
gf	-188.97	kJ/mol	Joback Method
hf	-291.08	kJ/mol	Joback Method
hfus	11.81	kJ/mol	Joback Method
hvap	48.70 ± 1.20	kJ/mol	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.26 ± 0.03	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.834		Crippen Method
mcvol	93.370	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpola	916.00		NIST Webbook
rinpola	925.00		NIST Webbook
rinpola	916.00		NIST Webbook
rinpola	910.60		NIST Webbook
ripola	1367.00		NIST Webbook
tb	430.00	K	NIST Webbook
tb	430.20	K	NIST Webbook

tc	613.45	K	Joback Method
tf	230.41	K	Joback Method
vc	0.355	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.33	J/mol×K	412.91	Joback Method
cpg	179.27	J/mol×K	446.33	Joback Method
cpg	188.77	J/mol×K	479.76	Joback Method
cpg	197.84	J/mol×K	513.18	Joback Method
cpg	206.49	J/mol×K	546.61	Joback Method
cpg	214.72	J/mol×K	580.03	Joback Method
cpg	222.53	J/mol×K	613.45	Joback Method
hvapt	48.70	kJ/mol	298.15	Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers

## Sources

Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers:	<a href="https://www.doi.org/10.1016/j.jct.2008.09.012">https://www.doi.org/10.1016/j.jct.2008.09.012</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C459609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C459609&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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