Benzene, 1-fluoro-4-methoxy-

Other names:	1-fluoro-4-methoxybenzene
	4-fluoroanisole
	4-fluoromethoxybenzene
	anisole, p-fluoro-
	p-Fluoromethoxybenzene
	p-Fluorophenyl methyl ether
	p-Methoxyfluorobenzene
	p-fluoroanisol
	p-fluoroanisole
Inchi:	InChI=1S/C7H7FO/c1-9-7-4-2-6(8)3-5-7/h2-5H,1H3
InchiKey:	VIPWUFMFHBIKQI-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	COc1ccc(F)cc1
Mol. weight [g/mol]:	126.13
CAS:	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
rinpol	916.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	910.60		NIST Webbook
rinpol	916.00		NIST Webbook
ripol	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	m3/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

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=C459609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers:	https://www.doi.org/10.1016/j.jct.2008.09.012

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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume