Benzene, 1-fluoro-2-methoxy-

Other names:	1-Fluoro-2-methoxybenzene
	2-fluoroanisole
	2-fluoromethoxybenzene
	anisole, o-fluoro-
	o-fluoroanisole
Inchi:	InChI=1S/C7H7FO/c1-9-7-5-3-2-4-6(7)8/h2-5H,1H3
InchiKey:	JIXDOBAQOWOUPA-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	COc1ccccc1F
Mol. weight [g/mol]:	126.13
CAS:	321-28-8

Physical Properties

Property code	Value	Unit	Source
affp	808.00	kJ/mol	NIST Webbook
basg	778.00	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	52.10 ± 1.10	kJ/mol	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	934.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	919.70		NIST Webbook
tb	427.70	K	NIST Webbook
tb	427.50 ± 0.50	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	52.20	kJ/mol	298.15	Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Diffusion coefficients of 2-fluoroanisole, 2-bromoanisole, ethylbenzene and 1,3-dimethylbenzene at infinite dilution in supercritical carbon dioxide:	https://www.doi.org/10.1016/j.fluid.2007.07.039
Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers:	https://www.doi.org/10.1016/j.jct.2008.09.012
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=C321288&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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