

3-FLUOROANISOLE

Other names:	3-fluoromethoxybenzene Benzene, 1-fluoro-3-methoxy- anisole, m-fluoro- m-fluoroanisole
Inchi:	InChI=1S/C7H7FO/c1-9-7-4-2-3-6(8)5-7/h2-5H,1H3
InchiKey:	MFJNOXOAIFNSBX-UHFFFAOYSA-N
Formula:	C7H7FO
SMILES:	COc1cccc(F)c1
Mol. weight [g/mol]:	126.13

Physical Properties

Property code	Value	Unit	Source
affp	825.00	kJ/mol	NIST Webbook
basg	795.00	kJ/mol	NIST Webbook
hf	-287.04	kJ/mol	Cheméo Relay (1.0)
hfus	11.81	kJ/mol	Joback Method
hvap	48.10 ± 1.10	kJ/mol	NIST Webbook
ie	8.41 ± 0.06	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-1.85		Cheméo Relay (1.0)
logp	1.834		Crippen Method
mcvol	93.370	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	925.00		NIST Webbook
rinpol	908.50		NIST Webbook
rinpol	908.50		NIST Webbook
tb	422.07	K	Cheméo Relay (1.0)
tc	631.29	K	Cheméo Relay (1.0)
tf	222.76	K	Cheméo Relay (1.0)

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	48.10	kJ/mol	298.15	Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.00	K	99.10	NIST Webbook
tbrp	431.20	K	99.10	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
Experimental and computational study on the molecular energetics of the three monofluoroanisole isomers:	https://www.doi.org/10.1016/j.jct.2008.09.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C456495&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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