M-FLUOROBENZAMIDE

Other names:	3-fluorobenzamide
	Benzamide, 3-fluoro-
	Benzamide, m-fluoro-
Inchi:	InChI=1S/C7H6FNO/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H2,9,10)
InchiKey:	YPIGHNIIXYSPKF-UHFFFAOYSA-N
Formula:	C7H6FNO
SMILES:	NC(=O)c1cccc(F)c1
Mol. weight [g/mol]:	139.13

Physical Properties

Property code	Value	Unit	Source
affp	877.20	kJ/mol	NIST Webbook
basg	846.30	kJ/mol	NIST Webbook
hf	-346.62	kJ/mol	Cheméo Relay (1.0)
hfus	21.50	kJ/mol	Thermodynamic Study of the Three Fluorobenzamides: Vapor Pressures, Phase Diagrams, and Hydrogen Bonds
hvap	64.05	kJ/mol	Cheméo Relay (1.0)
ie	9.60	eV	NIST Webbook
log10ws	-1.75		Cheméo Relay (1.0)
logp	0.925		Crippen Method
mcvol	99.050	ml/mol	McGowan Method
tb	501.65	K	Cheméo Relay (1.0)
tf	329.23	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.94	J/mol×K	516.89	Joback Method
cpg	218.62	J/mol×K	554.53	Joback Method
cpg	227.65	J/mol×K	592.18	Joback Method
cpg	236.05	J/mol×K	629.82	Joback Method

cpg	243.86	J/mol×K	667.47	Joback Method
cpg	251.10	J/mol×K	705.11	Joback Method
cpg	257.80	J/mol×K	742.75	Joback Method

Sources

Cheméo Relay (1.0, beta):

Thermodynamic Study of the Three Fluorobenzamides: Vapor Pressures, Phase Diagrams, and Hydrogen Bonds: https://www.doi.org/10.1021/je100801s

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C455378&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point