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
CAS:	455-37-8

Physical Properties

Property code	Value	Unit	Source
affp	877.20	kJ/mol	NIST Webbook
basg	846.30	kJ/mol	NIST Webbook
gf	-146.44	kJ/mol	Joback Method
hf	-237.65	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Thermodynamic Study of the Three Fluorobenzamides: Vapor Pressures, Phase Diagrams, and Hydrogen Bonds
hvap	50.68	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	0.925		Crippen Method
mcvol	99.050	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
tb	516.89	K	Joback Method
tc	742.75	K	Joback Method
tf	341.37	K	Joback Method
vc	0.372	m3/kmol	Joback Method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C455378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Study of the Three Fluorobenzamides: Vapor Pressures, Phase Diagrams, and Hydrogen Bonds:	https://www.doi.org/10.1021/je100801s
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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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