

Acetanilide, 4'-fluoro-

Other names:	4'-Fluoroacetanilide 4-Fluoroacetanilide Acetamide, N-(4-fluorophenyl)- N-(4-fluorophenyl)acetamide p-Fluoroacetanilide
Inchi:	InChI=1S/C8H8FNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)
InchiKey:	JHEFOJNPLXSWNZ-UHFFFAOYSA-N
Formula:	C8H8FNO
SMILES:	CC(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]:	153.15
CAS:	351-83-7

Physical Properties

Property code	Value	Unit	Source
chs	-4094.00	kJ/mol	NIST Webbook
gf	-115.08	kJ/mol	Joback Method
hf	-238.61	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	48.70	kJ/mol	Joback Method
ie	8.20 ± 0.03	eV	NIST Webbook
log10ws	-1.78		Aqueous Solubility Prediction Method
log10ws	-1.78		Estimated Solubility Method
logp	1.784		Crippen Method
mvol	113.140	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	517.41	K	Joback Method
tc	729.82	K	Joback Method
tf	322.04	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	242.65	J/mol×K	517.41	Joback Method
cpg	253.72	J/mol×K	552.81	Joback Method
cpg	264.12	J/mol×K	588.21	Joback Method
cpg	273.86	J/mol×K	623.61	Joback Method
cpg	282.97	J/mol×K	659.01	Joback Method
cpg	291.48	J/mol×K	694.41	Joback Method
cpg	299.41	J/mol×K	729.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C351837&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
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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