4-Fluoroacetanilide

Other names: 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]: 153.16

Physical Properties

Property code	Value	Unit	Source
chs	-4094.00	kJ/mol	NIST Webbook
hfus	19.91	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
mcvol	113.140	ml/mol	McGowan Method
tb	514.78	K	Cheméo Relay (1.0)
tf	351.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion 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