

4'-Fluoro-2'-nitroacetanilide

Other names:	4-Fluoro-2-nitroacetanilide
Inchi:	InChI=1S/C8H7FN2O3/c1-5(12)10-7-3-2-6(9)4-8(7)11(13)14/h2-4H,1H3,(H,10,12)
InchiKey:	UZBZEUCQENVPQB-UHFFFAOYSA-N
Formula:	C8H7FN2O3
SMILES:	CC(=O)Nc1ccc(F)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	198.15
CAS:	448-39-5

Physical Properties

Property code	Value	Unit	Source
chs	-3917.00	kJ/mol	NIST Webbook
gf	-89.16	kJ/mol	Joback Method
hf	-260.84	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	65.96	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.692		Crippen Method
mcvol	130.560	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	674.23	K	Joback Method
tc	912.12	K	Joback Method
tf	478.17	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.64	J/mol×K	674.23	Joback Method
cpg	336.51	J/mol×K	713.88	Joback Method
cpg	345.61	J/mol×K	753.53	Joback Method
cpg	353.96	J/mol×K	793.18	Joback Method
cpg	361.59	J/mol×K	832.82	Joback Method
cpg	368.54	J/mol×K	872.47	Joback Method
cpg	374.85	J/mol×K	912.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C448395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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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