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

Physical Properties

Property code	Value	Unit	Source
chs	-3917.00	kJ/mol	NIST Webbook
hfus	30.88	kJ/mol	Joback Method
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-2.81		Cheméo Relay (1.0)
logp	1.692		Crippen Method
mcvol	130.560	ml/mol	McGowan Method
tb	549.71	K	Cheméo Relay (1.0)
tf	383.41	K	Cheméo Relay (1.0)

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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C448395&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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