

2,4-Difluoro-6-nitroacetanilide

Other names: 2',4'-difluoro-6'-nitroacetanilide; Acetamide, N-(2,4-difluoro-6-nitrophenyl)-.

InChI: InChI=1S/C8H6F2N2O3/c1-4(13)11-8-6(10)2-5(9)3-7(8)12(14)15/h 2-3H,1H3,(H,11,13)

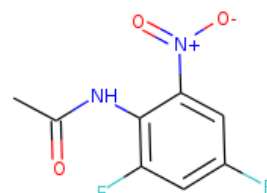
InChI Key: ZBECJQMWJBFRCL-UHFFFAOYSA-N

Formula: C8H6F2N2O3

SMILES: CC(=O)Nc1c(F)cc(F)cc1[N+](=O)[O-]

Molecular Weight: 216.14

CAS: 441-30-5



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-293.60	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-468.42	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	33.57	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	65.80	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	1.83		Crippen Method
P_c	3452.08	kPa	Joback Method
T_{boil}	678.48	K	Joback Method
T_c	906.48	K	Joback Method
T_{fus}	491.28	K	Joback Method
V_c	0.53	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	333.05	J/mol×K	678.48	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H6F2N2O3/c1-4\(13\)11-8-6\(10\)2-5\(9\)3-7\(8\)12\(14\)15/h2-3H,1H3,\(H,11,13\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C8H6F2N2O3/c1-4(13)11-8-6(10)2-5(9)3-7(8)12(14)15/h2-3H,1H3,(H,11,13))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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