Acetamide, N-(4-formylphenyl)-

Other names:	4'-Formylacetanilide
	4-(Acetalamino)benzaldehyde
	4-Acetamidobenzaldehyde
	4-Acetomidobenzaldehyde
	4-Acetylaminobenzaldehyde
	4-Formylacetanilide
	Acetanilide, 4'-formyl-
	Benzaldehyde, 4-acetamido-
	Micotiazone
	NSC 1701
	p-(Acetylamino)benzaldehyde
	p-Acetamidobenzaldehyde
	p-Acetaminobenzaldehyde
	p-Formylacetanilide
	para-Acetaminobenzaldehyde
Inchi:	InChI=1S/C9H9NO2/c1-7(12)10-9-4-2-8(6-11)3-5-9/h2-6H,1H3,(H,10,12)
InchiKey:	SKLUWKYNZNXSLX-UHFFFAOYSA-N
Formula:	C9H9NO2
SMILES:	CC(=O)Nc1ccc(C=O)cc1
Mol. weight [g/mol]:	163.17
CAS:	122-85-0

Physical Properties

Property code	Value	Unit	Source
gf	-11.37	kJ/mol	Joback Method
hf	-148.72	kJ/mol	Joback Method
hfus	21.71	kJ/mol	Joback Method
hvap	58.47	kJ/mol	Joback Method
log10ws	-1.58		Aqueous Solubility Prediction Method
logp	1.458		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
tb	589.68	K	Joback Method
tc	812.41	K	Joback Method
tf	430.82	K	Aqueous Solubility Prediction Method

vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.04	J/mol×K	589.68	Joback Method
cpg	304.13	J/mol×K	626.80	Joback Method
cpg	314.46	J/mol×K	663.92	Joback Method
cpg	324.07	J/mol×K	701.04	Joback Method
cpg	332.99	J/mol×K	738.16	Joback Method
cpg	341.25	J/mol×K	775.29	Joback Method
cpg	348.88	J/mol×K	812.41	Joback Method
hsubt	99.00	kJ/mol	337.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C122850&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

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
hsubt: Enthalpy of sublimation at a given temperature
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