Benzoic acid, 3-(acetylamino)-

Other names:	3-(acetylamino)benzoic acid
	3-acetamidobenzoic acid
	Acetyl-m-aminobenzoic acid
	Benzoic acid, m-acetamido-
	N-Acetyl-m-aminobenzoic acid
	NSC 4001
	m-Acetamidobenzoic acid
	m-Acetamino benzoic acid
	m-Acetylaminobenzoic acid
Inchi:	InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-3-7(5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
InchiKey:	RGDPZMQZWZMONQ-UHFFFAOYSA-N
Formula:	C9H9NO3
SMILES:	CC(O)=Nc1cccc(C(=O)O)c1
Mol. weight [g/mol]:	179.17
CAS:	587-48-4

Physical Properties

Property code	Value	Unit	Source
hf	-348.64	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
hfus	39.40	kJ/mol	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
hvap	82.06	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.993		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	751.77	K	Joback Method
tc	960.00	K	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Partial molar volumes of some drug and pro-drug substances in 1-octanol at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2009.10.002
Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids:	https://www.doi.org/10.1016/j.jct.2015.02.010
Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures:	https://www.doi.org/10.1016/j.tca.2014.03.019
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C587484&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature