# 2-acetamidobenzoic acid

Other names: N-acetylanthranilic acid

o-acetamidobenzoic acid

Inchi: InChl=1S/C9H9NO3/c1-6(11)10-8-5-3-2-4-7(8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)

InchiKey: QSACCXVHEVWNMX-UHFFFAOYSA-N

Formula: C9H9NO3

SMILES: CC(=O)Nc1ccccc1C(=O)O

Mol. weight [g/mol]: 179.18

## **Physical Properties**

gf       -177.59       kJ/mol       Joback Method         hf       -327.95       kJ/mol       Joback Method         hfus       29.32       kJ/mol       Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acidi isomers: Studying sublimation and fusion processes and their connection with crystal structures         hfus       49.40       kJ/mol       Acetamidobenzoic acidi isomers: Studying sublimation and fusion processes and their connection with crystal structures         hvap       75.17       kJ/mol       Joback Method         log10ws       -1.73       Crippen Method         logp       1.343       Crippen Method         mcvol       132.900       ml/mol       McGowan Method         pc       4244.08       kPa       Joback Method         tb       687.07       K       Joback Method         tf       458.40       K       Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures         tf       455.11       K       Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids         vc       0.497       m3/kmol       Joback Method	Property code	Value	Unit	Source
hfus 29.32 kJ/mol Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids  hfus 49.40 kJ/mol Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  hvap 75.17 kJ/mol Joback Method  log10ws -1.73 Crippen Method  logp 1.343 Crippen Method  mcvol 132.900 ml/mol McGowan Method  pc 4244.08 kPa Joback Method  tb 687.07 K Joback Method  tc 898.02 K Joback Method  tf 458.40 K Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  tf 455.11 K Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	gf	-177.59	kJ/mol	Joback Method
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isomers: Studying sublimation and fusion processes and their connection with crystal structures  hvap 75.17 kJ/mol Joback Method log10ws -1.73 Crippen Method logp 1.343 Crippen Method mcvol 132.900 ml/mol McGowan Method pc 4244.08 kPa Joback Method tb 687.07 K Joback Method tc 898.02 K Joback Method tf 458.40 K Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  tf 455.11 K Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	hfus	29.32	kJ/mol	of sublimation of the ortho and meta isomers of acetoxy and acetamido
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logp 1.343 Crippen Method mcvol 132.900 ml/mol McGowan Method pc 4244.08 kPa Joback Method tb 687.07 K Joback Method tc 898.02 K Joback Method  tf 458.40 K Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  tf 455.11 K Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	hvap	75.17	kJ/mol	Joback Method
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isomers: Studying sublimation and fusion processes and their connection with crystal structures  If 455.11 K Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	tc	898.02	K	Joback Method
of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	tf	458.40	K	isomers: Studying sublimation and fusion processes and their connection with crystal
vc 0.497 m3/kmol Joback Method	tf	455.11	К	of sublimation of the ortho and meta isomers of acetoxy and acetamido
	VC	0.497	m3/kmol	Joback Method

# **Temperature Dependent Properties**

Property code	Value	Unit	Temperature [K]	Source	
cpg	380.73	J/mol×K	898.02	Joback Method	
cpg	374.62	J/mol×K	862.86	Joback Method	
cpg	367.97	J/mol×K	827.70	Joback Method	
cpg	360.77	J/mol×K	792.54	Joback Method	
cpg	352.97	J/mol×K	757.39	Joback Method	
cpg	344.57	J/mol×K	722.23	Joback Method	
cpg	335.53	J/mol×K	687.07	Joback Method	
psub	3.73e-04	kPa	381.29	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	7.80e-04	kPa	387.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	8.40e-04	kPa	389.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	8.30e-05	kPa	367.17	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.09e-04	kPa	369.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	

1.60e-04	kPa	373.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
2.07e-04	kPa	375.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
2.48e-04	kPa	377.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
3.05e-04	kPa	379.19	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
3.85e-04	kPa	381.29	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
5.77e-04	kPa	385.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
6.97e-04	kPa	387.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
	2.07e-04  2.48e-04  3.05e-04  5.77e-04	2.07e-04 kPa  2.48e-04 kPa  3.05e-04 kPa  5.77e-04 kPa	2.07e-04	properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids  2.07e-04

psub	8.29e-04	kPa	389.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	8.30e-05	kPa	367.17	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.08e-04	kPa	369.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.28e-04	kPa	371.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	2.10e-04	kPa	375.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	2.55e-04	kPa	377.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	3.03e-04	kPa	379.19	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	

psub	5.74e-04	kPa	385.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	5.61e-04	kPa	385.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	7.11e-04	kPa	387.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	8.40e-04	kPa	389.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.66e-05	kPa	344.70	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures	
psub	3.37e-05	kPa	351.30	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures	
psub	5.58e-05	kPa	357.30	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures	

psub	1.11e-04	kPa	363.50	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
psub	1.16e-04	kPa	363.80	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
psub	1.38e-04	kPa	366.20	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
psub	2.35e-04	kPa	369.70	Acetamidobenzoic    acid isomers:    Studying    sublimation and    fusion processes    and their    connection with    crystal structures
psub	2.43e-04	kPa	371.00	Acetamidobenzoic    acid isomers:     Studying    sublimation and    fusion processes     and their    connection with    crystal structures
psub	2.89e-04	kPa	373.50	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
psub	5.55e-04	kPa	377.40	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures

psub 5.71e-04 kPa 380.00  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 9.48e-04 kPa 383.80  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 1.17e-03 kPa 387.20  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 1.52e-03 kPa 390.40  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 1.98e-03 kPa 390.40  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 1.98e-03 kPa 393.50  Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures  Psub 4.38e-04 kPa 383.16  Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acid somers: Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acid somers: Sublimation of the ortho and meta isomers of acetoxy and acetamido a					
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properties of sublimation of the ortho and meta isomers of acetoxy and acetamido	psub	4.38e-04	kPa	383.16	properties of sublimation of the ortho and meta isomers of acetoxy and acetamido
Denzoic acids	psub	3.78e-04	kPa	381.29	properties of sublimation of the ortho and meta isomers of acetoxy and

psub	3.08e-04	kPa	379.19	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	2.58e-04	kPa	377.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.63e-04	kPa	373.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	1.06e-04	kPa	369.28	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	
psub	8.30e-05	kPa	367.17	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids	

#### **Sources**

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen\_log10ws

https://www.doi.org/10.1016/j.jct.2015.02.010 Thermodynamic properties of sublimation of the ortho and meta sertems of the ortho and meta sertems of bearing arid in the interest of bearing and fusion processes and their connection with crystal structures: McGowan Method: https://www.doi.org/10.1016/j.tca.2014.03.019 https://en.wikipedia.org/wiki/Joback\_method

http://link.springer.com/article/10.1007/BF02311772

### Legend

**cpg:** Ideal gas heat capacity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

pc: Critical Pressure

**psub:** Sublimation pressure

**tb:** Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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