

2-acetamidobenzoic acid

Other names:	N-acetylanthranilic acid o-acetamidobenzoic acid
Inchi:	InChI=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

Property code	Value	Unit	Source
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 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
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.53	J/molxK	687.07	Joback Method
cpg	344.57	J/molxK	722.23	Joback Method
cpg	352.97	J/molxK	757.39	Joback Method
cpg	360.77	J/molxK	792.54	Joback Method
cpg	367.97	J/molxK	827.70	Joback Method
cpg	374.62	J/molxK	862.86	Joback Method
cpg	380.73	J/molxK	898.02	Joback Method
psub	8.29e-04	kPa	389.15	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	1.63e-04	kPa	373.16	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	3.08e-04	kPa	379.19	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids

psub	3.78e-04	kPa	381.29	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	4.38e-04	kPa	383.16	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	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

psub	1.60e-04	kPa	373.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	2.07e-04	kPa	375.26	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	2.48e-04	kPa	377.16	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	3.05e-04	kPa	379.19	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	3.85e-04	kPa	381.29	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	5.77e-04	kPa	385.15	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
psub	6.97e-04	kPa	387.26	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	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	3.73e-04	kPa	381.29	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	393.50	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures

Sources

Thermodynamic properties of sublimation of the ortho and meta isomers of benzoic acid and acetamidobenzoic acid isomers. Studying sublimation and fusion processes and their connection with crystal structures: McGowan Method:
Crippen Method:
Crippen Method:

<https://www.doi.org/10.1016/j.jct.2015.02.010>
<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>
<http://pubs.acs.org/doi/abs/10.1021/ci990307I>
https://www.chemeo.com/doc/models/crippen_log10ws

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
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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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