

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	49.40	kJ/mol	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
hfus	29.32	kJ/mol	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
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	455.11	K	Thermodynamic properties of sublimation of the ortho and meta isomers of acetoxy and acetamido benzoic acids
tf	458.40	K	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
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

McGowan Method:

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

Crippen Method:

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

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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

<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

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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