O-ACETAMIDOBENZOIC ACID

Other names: 2-acetamidobenzoic acid
N-acetylanthranilic 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
hf	-487.52	kJ/mol	Cheméo Relay (1.0)
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	97.21	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-1.91		Cheméo Relay (1.0)
logp	1.343		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
tb	573.03	K	Cheméo Relay (1.0)
tc	858.80	K	Cheméo Relay (1.0)
tf	442.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.53	J/mol×K	687.07	Joback Method
cpg	344.57	J/mol×K	722.23	Joback Method

cpg	352.97	J/mol×K	757.39	Joback Method
cpg	360.77	J/mol×K	792.54	Joback Method
cpg	367.97	J/mol×K	827.70	Joback Method
cpg	374.62	J/mol×K	862.86	Joback Method
cpg	380.73	J/mol×K	898.02	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C89521

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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

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

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

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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