Acedoben

Other names:
4'-Carboxyacetanilide
4-Acetylaminobenzoic acid
4-Carboxyacetanilide
4-acetamidobenzoic acid
Benzoic acid, 4-(acetylamino)-
Benzoic acid, p-acetamido-
N-(4-Carboxyphenyl)acetic acid amide
N-Acetyl-p-aminobenzoic acid
NSC 4002
PAAB
benzoic acid, 4-acetamido-
p-Acetamidobenzoic acid
p-Acetaminobenzoic acid
p-Acetaminophenylcarboxylic acid
p-Acetoaminobenzoic acid
p-Acetylaminobenzoic acid
p-Carboxyacetanilide

Inchi: InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
InchiKey: QCXJEYYXVJIFCE-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: CC(=O)Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 179.17
CAS: 556-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-177.59	kJ/mol	Joback Method
hf	-327.95	kJ/mol	Joback Method
hfus	34.20	kJ/mol	Acetamidobenzoic acid isomers: Studying sublimation and fusion processes and their connection with crystal structures
hvap	75.17	kJ/mol	Joback Method
ie	8.70 ± 0.20	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	1.343		Crippen Method

mcvol	132.900	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	2008.00		NIST Webbook
tb	687.07	K	Joback Method
tc	898.02	K	Joback Method
tf	443.47	K	Joback Method
vc	0.497	m3/kmol	Joback Method

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

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

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

Partial molar volumes of some drug and pro-drug substances in 1-octanol 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

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=C556081&Units=SI

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

ie: Ionization energy

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

tf: Normal melting (fusion) point

vc: Critical Volume