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

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
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 at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2009.10.002

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