Benzoic acid, 4-amino-, methyl ester

Other names:	4-(Carbomethoxy)aniline
	4-(Methoxycarbonyl)aniline
	4-Aminobenzoic acid methyl ester
	4-aminobenzoic acid, methyl ester
	Benzoic acid, p-amino-, methyl ester
	Methyl 4-aminobenzoate
	Methyl aniline-4-carboxylate
	Methyl ester of 4-aminobenzoic acid
	Methyl ester of p-aminobenzoic acid
	Methyl p-aminobenzoate
	NSC 3783
	p-(Methoxycarbonyl)aniline
	p-Aminobenzoic acid methyl ester
Inchi:	InChI=1S/C8H9NO2/c1-11-8(10)6-2-4-7(9)5-3-6/h2-5H,9H2,1H3
InchiKey:	LZXXNPOYQCLXRS-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	COC(=O)c1ccc(N)cc1
Mol. weight [g/mol]:	151.16
CAS:	619-45-4

Physical Properties

Property code	Value	Unit	Source
affp	883.90	kJ/mol	NIST Webbook
basg	853.00	kJ/mol	NIST Webbook
gf	-48.21	kJ/mol	Joback Method
hf	-194.40	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids
hvap	56.14	kJ/mol	Joback Method
ie	8.08 ± 0.01	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	-1.20		Aqueous Solubility Prediction Method
logp	1.055		Crippen Method

mcvol	117.240	ml/mol	McGowan Method
pc	4072.51	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	562.92	K	Joback Method
tc	793.64	K	Joback Method
tf	384.40	K	Aqueous Solubility Prediction Method
tf	385.00 ± 1.00	K	NIST Webbook
tf	385.70 ± 0.50	K	NIST Webbook
tf	385.10 ± 0.50	K	NIST Webbook
tf	384.30 ± 0.50	K	NIST Webbook
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.72	J/mol×K	716.73	Joback Method
cpg	314.25	J/mol×K	755.19	Joback Method
cpg	264.93	J/mol×K	562.92	Joback Method
cpg	276.15	J/mol×K	601.37	Joback Method
cpg	286.68	J/mol×K	639.83	Joback Method
cpg	296.53	J/mol×K	678.28	Joback Method
cpg	322.15	J/mol×K	793.64	Joback Method
hfust	22.55	kJ/mol	385.10	NIST Webbook
hfust	22.55	kJ/mol	385.10	NIST Webbook

Sources

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

Thermodynamic study of phase transitions in methyl esters of ortho-, meta-, and para-aminobenzoic acids: https://www.doi.org/10.1016/j.jct.2012.04.006

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619454&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfust:	Enthalpy of fusion at a given temperature
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