4-Amino-3-methylbenzoic acid

Other names:	Benzoic acid, 4-amino-3-methyl-
Inchi:	InChI=1S/C8H9NO2/c1-5-4-6(8(10)11)2-3-7(5)9/h2-4H,9H2,1H3,(H,10,11)
InchiKey:	NHFKECPTBZZFBC-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	Cc1cc(C(=O)O)ccc1N
Mol. weight [g/mol]:	151.16
CAS:	2486-70-6

Physical Properties

Property code	Value	Unit	Source
gf	-89.66	kJ/mol	Joback Method
hf	-225.88	kJ/mol	Joback Method
hfus	20.62	kJ/mol	Joback Method
hsub	122.00 ± 2.60	kJ/mol	NIST Webbook
hvap	71.07	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.275		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	637.66	K	Joback Method
tc	853.80	K	Joback Method
tf	425.39	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.86	J/mol×K	781.76	Joback Method
cpg	323.68	J/mol×K	817.78	Joback Method
cpg	284.29	J/mol×K	637.66	Joback Method
cpg	293.26	J/mol×K	673.68	Joback Method
cpg	301.67	J/mol×K	709.71	Joback Method
cpg	309.53	J/mol×K	745.73	Joback Method
cpg	330.01	J/mol×K	853.80	Joback Method

hfust	21.77	kJ/mol	439.40	NIST Webbook
hsubt	119.80 ± 0.70	kJ/mol	375.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2486706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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