Benzamide, 3-amino-

Other names:	3-NH2-C6H4CONH2
	3-aminobenzamide
	Benzamide, m-amino-
	m-aminobenzamide
Inchi:	InChI=1S/C7H8N2O/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,8H2,(H2,9,10)
InchiKey:	GSCPDZHWVNUUFI-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	NC(=O)c1cccc(N)c1
Mol. weight [g/mol]:	136.15
CAS:	3544-24-9

Physical Properties

Property code	Value	Unit	Source
affp	900.90	kJ/mol	NIST Webbook
basg	869.90	kJ/mol	NIST Webbook
gf	114.82	kJ/mol	Joback Method
hf	-7.75	kJ/mol	Joback Method
hfus	19.53	kJ/mol	Joback Method
hvap	62.14	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.368		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	590.15	K	Joback Method
tc	837.19	K	Joback Method
tf	424.04	K	Joback Method
tt	352.40	K	Experimental and computational thermodynamic study of ortho- meta- and para-aminobenzamide
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	248.85	J/mol×K	590.15	Joback Method
cpg	259.00	J/mol×K	631.32	Joback Method
cpg	268.39	J/mol×K	672.50	Joback Method
cpg	277.04	J/mol×K	713.67	Joback Method
cpg	284.99	J/mol×K	754.84	Joback Method
cpg	292.28	J/mol×K	796.02	Joback Method
cpg	298.94	J/mol×K	837.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3544249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermodynamic study of ortho- meta- and- para-aminobenzamide:	https://www.doi.org/10.1016/j.jct.2012.12.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
tt:	Triple Point Temperature
vc:	Critical Volume

Latest version available from: