

3-Amino-5-nitrobenzoic acid

Other names:	Benzoic acid, 3-amino-5-nitro-
Inchi:	InChI=1S/C7H6N2O4/c8-5-1-4(7(10)11)2-6(3-5)9(12)13/h1-3H,8H2,(H,10,11)
InchiKey:	ZNVHAQRPXAQKRU-UHFFFAOYSA-N
Formula:	C7H6N2O4
SMILES:	Nc1cc(C(=O)O)cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	182.13
CAS:	618-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-62.53	kJ/mol	Joback Method
hf	-216.00	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	85.43	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	0.875		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
tb	766.62	K	Joback Method
tc	1006.55	K	Joback Method
tf	557.73	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.02	J/mol×K	766.62	Joback Method
cpg	320.05	J/mol×K	806.61	Joback Method
cpg	326.45	J/mol×K	846.60	Joback Method
cpg	332.26	J/mol×K	886.59	Joback Method
cpg	337.50	J/mol×K	926.58	Joback Method
cpg	342.20	J/mol×K	966.57	Joback Method
cpg	346.41	J/mol×K	1006.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C618848&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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