Benzamide, 3-nitro-

Other names: 3-nitrobenzamide
Benzamide, m-nitro-
m-nitrobenzamide
Inchi: InChI=1S/C7H6N2O3/c8-7(10)5-2-1-3-6(4-5)9(11)12/h1-4H,(H2,8,10)
InchiKey: KWAYEPXDGHYGRW-UHFFFAOYSA-N
Formula: C7H6N2O3
SMILES: NC(=O)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 166.13
CAS: 645-09-0

Physical Properties

Property code	Value	Unit	Source
affp	854.20	kJ/mol	NIST Webbook
basg	823.20	kJ/mol	NIST Webbook
gf	83.92	kJ/mol	Joback Method
hf	-52.30	kJ/mol	Joback Method
hfus	24.58	kJ/mol	Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis
hvap	68.09	kJ/mol	Joback Method
ie	10.28	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	0.694		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	4809.16	kPa	Joback Method
tb	585.70	K	NIST Webbook
tc	933.02	K	Joback Method
tf	484.39	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	278.75	J/mol×K	669.46	Joback Method
cpg	288.09	J/mol×K	713.39	Joback Method
cpg	296.56	J/mol×K	757.31	Joback Method
cpg	304.23	J/mol×K	801.24	Joback Method
cpg	311.14	J/mol×K	845.17	Joback Method
cpg	317.33	J/mol×K	889.09	Joback Method
cpg	322.86	J/mol×K	933.02	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gas phase enthalpies of formation of nitrobenzamides using combustion calorimetry and thermal analysis:	https://www.doi.org/10.1016/j.jct.2014.07.006
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=C645090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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