3-Hydroxy-4-nitrobenzoic acid

Other names:	4-Nitro-3-hydroxybenzoic acid
	Benzoic acid, 3-hydroxy-4-nitro-
Inchi:	InChI=1S/C7H5NO5/c9-6-3-4(7(10)11)1-2-5(6)8(12)13/h1-3,9H,(H,10,11)
InchiKey:	XLDLRRGZWIEEHT-UHFFFAOYSA-N
Formula:	C7H5NO5
SMILES:	O=C(O)c1ccc([N+](=O)[O-])c(O)c1
Mol. weight [g/mol]:	183.12
CAS:	619-14-7

Physical Properties

Property code	Value	Unit	Source
gf	-273.97	kJ/mol	Joback Method
hf	-415.63	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	87.14	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	0.999		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	769.73	K	Joback Method
tc	1010.82	K	Joback Method
tf	573.67	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.18	J/mol×K	769.73	Joback Method
cpg	308.59	J/mol×K	809.91	Joback Method
cpg	314.62	J/mol×K	850.09	Joback Method
cpg	320.35	J/mol×K	890.28	Joback Method
cpg	325.89	J/mol×K	930.46	Joback Method
cpg	331.30	J/mol×K	970.64	Joback Method
cpg	336.69	J/mol×K	1010.82	Joback Method

Sources

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=C619147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/18-773-4/3-Hydroxy-4-nitrobenzoic-acid.pdf
Generated by Cheméo on 2024-10-12 06:16:45.488064589 +0000 UTC m=+3294668.125033838.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.