4-Hydroxy-3-nitrobenzaldehyde

Other names: Benzaldehyde, 4-hydroxy-3-nitro-
Inchi: InChI=1S/C7H5NO4/c9-4-5-1-2-7(10)6(3-5)8(11)12/h1-4,10H
InchiKey: YTHJCZRFJGXPTL-UHFFFAOYSA-N
Formula: C7H5NO4
SMILES: O=Cc1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 167.12
CAS: 3011-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-107.75	kJ/mol	Joback Method
hf	-236.40	kJ/mol	Joback Method
hfus	26.97	kJ/mol	Joback Method
hvap	70.44	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.113		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
pc	5577.49	kPa	Joback Method
tb	672.34	K	Joback Method
tc	932.41	K	Joback Method
tf	504.92	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.69	J/mol×K	672.34	Joback Method
cpg	277.54	J/mol×K	715.68	Joback Method
cpg	284.76	J/mol×K	759.03	Joback Method
cpg	291.46	J/mol×K	802.37	Joback Method
cpg	297.73	J/mol×K	845.72	Joback Method
cpg	303.70	J/mol×K	889.06	Joback Method
cpg	309.47	J/mol×K	932.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3011345&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
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