Benzaldehyde, 5-hydroxy-2-nitro-

Other names:	6-Nitro-3-hydroxybenzaldehyde
	Benzaldehyde, 5-hydroxy-2-nitro-
	3-Formyl-4-nitrophenol
Inchi:	InChI=1S/C7H5NO4/c9-4-5-3-6(10)1-2-7(5)8(11)12/h1-4,10H
InchiKey:	XLYPHUGUKGMURE-UHFFFAOYSA-N
Formula:	C7H5NO4
SMILES:	O=Cc1cc(O)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	167.12

Physical Properties

Property code	Value	Unit	Source
hf	-217.23	kJ/mol	Cheméo Relay (1.0)
hfus	26.97	kJ/mol	Joback Method
hvap	86.65	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-2.02		Cheméo Relay (1.0)
logp	1.113		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
tb	568.26	K	Cheméo Relay (1.0)
tf	384.91	K	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42454068&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point