3-Cyanobenzaldehyde

Other names: Benzonitrile, 3-formyl-
m-formylbenzonitrile
Inchi: InChI=1S/C8H5NO/c9-5-7-2-1-3-8(4-7)6-10/h1-4,6H
InchiKey: HGZJJKZPPMFIBU-UHFFFAOYSA-N
Formula: C8H5NO
SMILES: N#Cc1cccc(C=O)c1
Mol. weight [g/mol]: 131.13
CAS: 24964-64-5

Physical Properties

Property code	Value	Unit	Source
ea	1.01 ± 0.10	eV	NIST Webbook
ea	0.97 ± 0.09	eV	NIST Webbook
gf	152.92	kJ/mol	Joback Method
hf	95.91	kJ/mol	Joback Method
hfus	13.92	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.371		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	483.20	K	NIST Webbook
tc	800.60	K	Joback Method
tf	325.85	K	Joback Method
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.47	J/mol×K	564.84	Joback Method
cpg	221.04	J/mol×K	604.13	Joback Method
cpg	229.00	J/mol×K	643.43	Joback Method
cpg	236.37	J/mol×K	682.72	Joback Method
cpg	243.18	J/mol×K	722.02	Joback Method

cpg	249.46	J/mol×K	761.31	Joback Method
cpg	255.23	J/mol×K	800.60	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24964645&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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