BENZONITRILE, 4-FORMYL-

Other names:	4-Cyanobenzaldehyde
	4-Formylbenzonitrile
	Benzaldehyde, p-cyano-
	Benzonitrile, p-formyl-
	NSC 5091
	Terephthalaldehydonitrile
	USAF KF-1
	p-Cyanobenzaldehyde
	p-Cyanobenzenecarboxaldehyde
	p-Formylbenzonitrile
Inchi:	InChI=1S/C8H5NO/c9-5-7-1-3-8(6-10)4-2-7/h1-4,6H
InchiKey:	WZWIQYMTQZCSKI-UHFFFAOYSA-N
Formula:	C8H5NO
SMILES:	N#Cc1ccc(C=O)cc1
Mol. weight [g/mol]:	131.13

Physical Properties

Property code	Value	Unit	Source
af	0.4672		Cheméo Relay (1.0)
affp	796.90	kJ/mol	NIST Webbook
basg	766.30	kJ/mol	NIST Webbook
ea	1.22 ± 0.09	eV	NIST Webbook
ea	1.17 ± 0.09	eV	NIST Webbook
gf	152.92	kJ/mol	Joback Method
hf	105.75	kJ/mol	Cheméo Relay (1.0)
hfus	13.92	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	NIST Webbook
log10ws	-1.55		Cheméo Relay (1.0)
logp	1.371		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	524.01	K	Cheméo Relay (1.0)
tc	783.41	K	Cheméo Relay (1.0)
tf	357.46	K	Cheméo Relay (1.0)

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	1.60	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C105077&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

affp: Proton affinity

basg: Gas basicity

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point