2-CYANOBENZALDEHYDE

Other names: o-Cyanobenzaldehyde
Inchi: InChI=1S/C8H5NO/c9-5-7-3-1-2-4-8(7)6-10/h1-4,6H
InchiKey: QVTPWONEVZJCCS-UHFFFAOYSA-N
Formula: C8H5NO
SMILES: N#Cc1ccccc1C=O
Mol. weight [g/mol]: 131.13

Physical Properties

Property code	Value	Unit	Source
hf	101.23	kJ/mol	Cheméo Relay (1.0)
hfus	13.92	kJ/mol	Joback Method
hvap	65.95	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-1.56		Cheméo Relay (1.0)
logp	1.371		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
tb	525.70	K	Cheméo Relay (1.0)
tc	797.76	K	Cheméo Relay (1.0)
tf	318.42	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

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7468679&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point