

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
CAS:	7468-67-9

Physical Properties

Property code	Value	Unit	Source
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	564.84	K	Joback Method
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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7468679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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