

3-Cyanobenzyl radical

Inchi:	InChI=1S/C8H6N/c1-7-3-2-4-8(5-7)6-9/h2-5H,1H2
InchiKey:	SCLFNIOYFAYJST-UHFFFAOYSA-N
Formula:	C8H6N
SMILES:	[CH2]c1cccc(C#N)c1
Mol. weight [g/mol]:	116.14
CAS:	61142-85-6

Physical Properties

Property code	Value	Unit	Source
gf	304.82	kJ/mol	Joback Method
hf	237.30	kJ/mol	Joback Method
hfus	13.32	kJ/mol	Joback Method
hvap	46.67	kJ/mol	Joback Method
ie	8.60 ± 0.10	eV	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.740		Crippen Method
mcvol	99.050	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	515.48	K	Joback Method
tc	744.40	K	Joback Method
tf	300.22	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.45	J/mol×K	515.48	Joback Method
cpg	202.36	J/mol×K	553.63	Joback Method
cpg	210.57	J/mol×K	591.79	Joback Method
cpg	218.13	J/mol×K	629.94	Joback Method
cpg	225.11	J/mol×K	668.09	Joback Method
cpg	231.58	J/mol×K	706.24	Joback Method
cpg	237.60	J/mol×K	744.40	Joback Method

Sources

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=C61142856&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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