Benzene, (isocyanomethyl)-

Other names:	Benzyl isocyanide
	Benzyl isonitrile
Inchi:	InChI=1S/C8H7N/c1-9-7-8-5-3-2-4-6-8/h2-6H,7H2
InchiKey:	RIWNFZUWWRVGEU-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	[C-]#[N+]Cc1ccccc1
Mol. weight [g/mol]:	117.15
CAS:	10340-91-7

Physical Properties

Property code	Value	Unit	Source
chl	-4373.74	kJ/mol	NIST Webbook
gf	262.07	kJ/mol	Joback Method
hf	192.96	kJ/mol	Joback Method
hfus	12.02	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
ie	9.61 ± 0.05	eV	NIST Webbook
ie	9.47	eV	NIST Webbook
log10ws	-4.54		Crippen Method
logp	2.106		Crippen Method
mcvol	101.200	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	511.20	K	Joback Method
tc	742.87	K	Joback Method
tf	271.33	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.73	J/mol×K	511.20	Joback Method
cpg	212.16	J/mol×K	549.81	Joback Method
cpg	221.87	J/mol×K	588.42	Joback Method
cpg	230.90	J/mol×K	627.04	Joback Method

cpg	239.28	J/mol×K	665.65	Joback Method
cpg	247.04	J/mol×K	704.26	Joback Method
cpg	254.23	J/mol×K	742.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10340917&Units=SI
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

Legend

chl:	Standard liquid enthalpy of combustion
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