Propanenitrile, 3,3'-iminobis-

Other names:	Bis(2-cyanoethyl)amine
	Propionitrile, 3,3'-iminodi-
	«beta»,«beta»'-Iminodipropionitrile
	Bis(«beta»-cyanoethyl)amine
	BBCE
	Di(2-Cyanoethyl)amine
	Ethanamine, 2-cyano-N-(2-cyanoethyl)-
	IDPN
	N,N-Bis(2-Cyanoethyl)amine
	3,3'-Iminobis(propionitrile)
	3,3'-Iminobis[propanenitrile]
	3,3'-Iminodipropionitrile
	HN(CH2CH2CN)2
	Iminodipropionitrile
	Diethylamine, 2,2'-dicyano-
	Imino-«beta»,«beta»'-dipropionitrile
	Iminodipropanenitrile
	USAF A-8564
	3,3'-Iminodipropanenitrile
	Bis-(2-kyanethyl)amin
	Di(2-cianoetil)ammina
	2341 I.S.
	NSC 7770
	3,3'-iminodipropiononitrile
Inchi:	InChI=1S/C6H9N3/c7-3-1-5-9-6-2-4-8/h9H,1-2,5-6H2
InchiKey:	SBAJRGRUGUQKAF-UHFFFAOYSA-N
Formula:	C6H9N3
SMILES:	N#CCCNCCC#N
Mol. weight [g/mol]:	123.16
CAS:	111-94-4

Physical Properties

Property code	Value	Unit	Source
gf	355.39	kJ/mol	Joback Method
hf	216.06	kJ/mol	Joback Method
hfus	19.41	kJ/mol	Joback Method

hvap	56.34	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.403		Crippen Method
mcvol	108.140	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	591.01	K	Joback Method
tc	799.30	K	Joback Method
tf	267.45 ± 0.30	K	NIST Webbook
tf	266.49 ± 0.20	K	NIST Webbook
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.29	J/mol×K	591.01	Joback Method
cpg	256.35	J/mol×K	625.72	Joback Method
cpg	263.98	J/mol×K	660.44	Joback Method
cpg	271.19	J/mol×K	695.15	Joback Method
cpg	277.99	J/mol×K	729.87	Joback Method
cpg	284.41	J/mol×K	764.58	Joback Method
cpg	290.44	J/mol×K	799.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	478.20	K	3.30	NIST Webbook
tbrp	408.00 ± 1.00	K	0.10	NIST Webbook
tbrp	407.50 ± 0.50	K	0.10	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C111944&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

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