N,N-Bis(2-cyanoethyl)aniline

Other names: N,N-Bis-cyanoethylaniline
N,N-Bis(2-cyanoethyl)aniline
Propanenitrile, 3,3'-(phenylimino)bis-
(«beta»-Cyanoethyl)benzylamine
Aniline, N,N-bis(2-cyanoethyl)-
Aniline, N,N-dicyanoethyl-
Bis(2-cyanoethyl)phenylamine
N,N-Bis(«beta»-cyanoethyl)aniline
Propionitrile, 3,3'-(phenylimino)di-
NSC 108353
3,3'-(phenylimino)bispropiononitrile

Inchi: InChI=1S/C12H13N3/c13-8-4-10-15(11-5-9-14)12-6-2-1-3-7-12/h1-3,6-7H,4-5,10-11H2

InchiKey: NSVHSAUVIFTVPN-UHFFFAOYSA-N

Formula: C12H13N3

SMILES: N#CCCN(CCC#N)c1ccccc1

Mol. weight [g/mol]: 199.26

Physical Properties

Property code	Value	Unit	Source
hf	308.33	kJ/mol	Cheméo Relay (1.0)
hfus	26.91	kJ/mol	Joback Method
hvap	89.78	kJ/mol	Cheméo Relay (1.0)
ie	8.71	eV	Cheméo Relay (1.0)
log10ws	-2.67		Cheméo Relay (1.0)
logp	2.320		Crippen Method
mcvol	168.920	ml/mol	McGowan Method
tb	607.76	K	Cheméo Relay (1.0)
tf	341.76	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.97	J/mol×K	717.24	Joback Method
cpg	453.50	J/mol×K	754.71	Joback Method

cpg	464.19	J/mol×K	792.18	Joback Method
cpg	474.11	J/mol×K	829.65	Joback Method
cpg	483.29	J/mol×K	867.13	Joback Method
cpg	491.81	J/mol×K	904.60	Joback Method
cpg	499.72	J/mol×K	942.07	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1555664&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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):

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
tf: Normal melting (fusion) point