

3,3'-(Phenylimino)dipropionitrile

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)bispropionitrile
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:	<chem>N#CCCN(CCC#N)c1ccccc1</chem>
Mol. weight [g/mol]:	199.25
CAS:	1555-66-4

Physical Properties

Property code	Value	Unit	Source
gf	539.71	kJ/mol	Joback Method
hf	342.81	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	67.58	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.320		Crippen Method
mcvol	168.920	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
tb	717.24	K	Joback Method
tc	942.07	K	Joback Method
tf	413.87	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	441.97	J/molxK	717.24	Joback Method
cpg	453.50	J/molxK	754.71	Joback Method
cpg	464.19	J/molxK	792.18	Joback Method
cpg	474.11	J/molxK	829.65	Joback Method
cpg	483.29	J/molxK	867.13	Joback Method
cpg	491.81	J/molxK	904.60	Joback Method
cpg	499.72	J/molxK	942.07	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C1555664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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