Propanenitrile, 3-(phenylamino)-

Other names:	(«beta»-Cyanoethyl)aniline
	2-Phenylaminopropionitrile
	3-(Phenylamino)propanenitrile
	3-Phenylamino-propionitrile
	3-anilinopropanenitrile
	3-anilinopropionitrile
	Aniline, N-beta-cyanoethyl-
	N-(2-Cyanoethyl)aniline
	N-(Cyanoethyl)aniline
	N-(«beta»-Cyanoethyl)aniline
	NSC 80663
	Propanenitrile, 3-anilino-
	Propionitrile, 3-anilino-
	«beta»-Anilinopropanenitrile
	«beta»-Anilinopropionitrile
Inchi:	InChI=1S/C9H10N2/c10-7-4-8-11-9-5-2-1-3-6-9/h1-3,5-6,11H,4,8H2
InchiKey:	FENJKTQEFUPECW-UHFFFAOYSA-N
Formula:	C9H10N2
SMILES:	N#CCCNc1ccccc1
Mol. weight [g/mol]:	146.19
CAS:	1075-76-9

Physical Properties

Property code	Value	Unit	Source
gf	359.88	kJ/mol	Joback Method
hf	225.79	kJ/mol	Joback Method
hfus	19.40	kJ/mol	Heat capacity and thermodynamic properties of N-(2-cyanoethyl) aniline (C9H10N2)
hvap	54.82	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.012		Crippen Method
mcvol	125.270	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	584.25	K	Joback Method
tc	810.87	K	Joback Method
tf	335.26	K	Joback Method

vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.07	J/mol×K	584.25	Joback Method
cpg	299.67	J/mol×K	622.02	Joback Method
cpg	310.48	J/mol×K	659.79	Joback Method
cpg	320.53	J/mol×K	697.56	Joback Method
cpg	329.85	J/mol×K	735.33	Joback Method
cpg	338.51	J/mol×K	773.10	Joback Method
cpg	346.52	J/mol×K	810.87	Joback Method
hfust	19.40	kJ/mol	218.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat capacity and thermodynamic properties of N-(2-cyanoethyl) aniline ($C_9H_{10}N_2$):	https://www.doi.org/10.1016/j.tca.2004.12.015
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=C1075769&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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