Propanenitrile, 3-(ethylphenylamino)-

Other names:	Propionitrile, 3-(N-ethylanilino)-
	N-«beta»-Cyanoethyl-N-ethylaminobenzene
	N-«beta»-Cyanoethyl-N-ethylaniline
	N-(Cyanoethyl)-N-ethylaniline
	N-(2-Cyanoethyl)-N-ethylaniline
	N-Ethyl-N-(«beta»-cyanoethyl)aniline
	N-Ethyl-N-(2-cyanoethyl)aniline
	N-Ethyl-N-cyanoethylaniline
	3-(Ethylphenylamino)propionitrile
	3-(N-Ethylanilino)propionitrile
	Aniline, N-ethyl-N-(2-cyanoethyl)-
	Aniline, N-(2-cyanoethyl)-N-ethyl-
	N-Ethyl-N-2-kyanethylanilin
	NSC 81243
	3-(N-ethylanilino)propiononitrile
Inchi:	InChI=1S/C11H14N2/c1-2-13(10-6-9-12)11-7-4-3-5-8-11/h3-5,7-8H,2,6,10H2,1H3
InchiKey:	WYRNRZQRKCXPLA-UHFFFAOYSA-N
Formula:	C11H14N2
SMILES:	CCN(CCC#N)c1ccccc1
Mol. weight [g/mol]:	174.24
CAS:	148-87-8

Physical Properties

Property code	Value	Unit	Source
gf	398.11	kJ/mol	Joback Method
hf	198.57	kJ/mol	Joback Method
hfus	22.81	kJ/mol	Joback Method
hvap	54.88	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.427		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
tb	592.28	K	Joback Method
tc	808.28	K	Joback Method
tf	337.61	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.02	J/mol×K	592.28	Joback Method
cpg	383.94	J/mol×K	628.28	Joback Method
cpg	396.94	J/mol×K	664.28	Joback Method
cpg	409.06	J/mol×K	700.28	Joback Method
cpg	420.37	J/mol×K	736.28	Joback Method
cpg	430.90	J/mol×K	772.28	Joback Method
cpg	440.71	J/mol×K	808.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C148878&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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume