Benzonitrile, p-(3-butyl-3-methyl-1-triazeno)-

Inchi: InChI=1S/C12H16N4/c1-3-4-9-16(2)15-14-12-7-5-11(10-13)6-8-12/h5-8H,3-4,9H2,1-2H3
InchiKey: WHJFWUCUNXMLSQ-CCEZHUSRSA-N
Formula: C12H16N4
SMILES: CCCCN(C)N=Nc1ccc(C#N)cc1
Mol. weight [g/mol]: 216.28
CAS: 116495-79-5

Physical Properties

Property code	Value	Unit	Source
hf	213.68	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.289		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
tb	769.34	K	Joback Method
tc	1000.47	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495795&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation 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