Butyronitrile, 2,3,3-trimethyl-2-(4-bromophenyldiazenyl)-

Other names: N-(4-Bromophenyl)-N'-(1,2,2-trimethyl-1-cyano-propyl)diazene
Inchi: InChI=1S/C13H16BrN3/c1-12(2,3)13(4,9-15)17-16-11-7-5-10(14)6-8-11/h5-8H,1-4H3
InchiKey: BOUQEKBWOQIMIL-UHFFFAOYSA-N
Formula: C13H16BrN3
SMILES: CC(C)(C)C(C)(C#N)N=Nc1ccc(Br)cc1
Mol. weight [g/mol]: 294.19
CAS: 40620-33-5

Physical Properties

Property code	Value	Unit	Source
hf	134.34	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.861		Crippen Method
mcvol	204.810	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	839.48	K	Joback Method
tc	1103.93	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40620335&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