

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

Other names:	N-(4-Nitrophenyl)-N'-(1,2,2-trimethyl-1-cyano-propyl)diazene
Inchi:	InChI=1S/C13H16N4O2/c1-12(2,3)13(4,9-14)16-15-10-5-7-11(8-6-10)17(18)19/h5-8H,1-
InchiKey:	ADUZTDVESOKFGH-UHFFFAOYSA-N
Formula:	C13H16N4O2
SMILES:	CC(C)(C)C(C)(C#N)N=Nc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	260.29
CAS:	40620-35-7

Physical Properties

Property code	Value	Unit	Source
hf	97.25	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.007		Crippen Method
mcvol	204.730	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
tb	925.16	K	Joback Method
tc	1195.36	K	Joback Method

Sources

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=C40620357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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