Benzoic acid, 2-(3-butyl-3-methyl-1-triazeno)-, hydrazide

Inchi: InChI=1S/C12H19N5O/c1-3-4-9-17(2)16-15-11-8-6-5-7-10(11)12(18)14-13/h5-8H,3-4,9,1

InchiKey: XPJQJEMAJZIYGG-FOCLMDBBSA-N

Formula: C12H19N5O

SMILES: CCCCN(C)N=Nc1ccccc1C(=O)NN

Mol. weight [g/mol]: 249.31

CAS: 116466-08-1

Physical Properties

Property code	Value	Unit	Source
hf	23.48	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.021		Crippen Method
mcvol	203.350	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
tb	843.83	K	Joback Method
tc	1074.05	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=C116466081&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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