Benzoic acid, 2-(3-cyclohexyl-3-methyltriazeno)-, methyl ester

Inchi: InChI=1S/C15H21N3O2/c1-18(12-8-4-3-5-9-12)17-16-14-11-7-6-10-13(14)15(19)20-2/h6
InchiKey: WBEQJYAIJWSKKY-WUKNDPDISA-N
Formula: C15H21N3O2
SMILES: COC(=O)c1ccccc1N=NN(C)C1CCCCC1
Mol. weight [g/mol]: 275.35
CAS: 116557-75-6

Physical Properties

Property code	Value	Unit	Source
hf	-203.60	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.736		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
tb	831.74	K	Joback Method
tc	1075.24	K	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116557756&Units=SI

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