Benzoic acid, o-(3,3-dimethyl-1-triazeno)-, methyl ester

Inchi: InChI=1S/C10H13N3O2/c1-13(2)12-11-9-7-5-4-6-8(9)10(14)15-3/h4-7H,1-3H3/b12-11+

InchiKey: BAGBQDMUYKXJIR-VAWYXSNFSA-N

Formula: C10H13N3O2

SMILES: COC(=O)c1ccccc1N=NN(C)C

Mol. weight [g/mol]: 207.23

CAS: 35967-28-3

Physical Properties

Property code	Value	Unit	Source
hf	-154.72	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.034		Crippen Method
mcvol	161.080	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
tb	697.79	K	Joback Method
tc	928.88	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=C35967283&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