Benzoic acid, 2-{3-[2-(diethylamino)ethyl]-3-methyltriazeno}-, methyl ester

Inchi: InChI=1S/C15H24N4O2/c1-5-19(6-2)12-11-18(3)17-16-14-10-8-7-9-13(14)15(20)21-4/h7
InchiKey: XPOKLMOUTMGTBB-WUKNDPDISA-N
Formula: C15H24N4O2
SMILES: CCN(CC)CCN(C)N=Nc1ccccc1C(=O)OC
Mol. weight [g/mol]: 292.38
CAS: 127909-49-3

Physical Properties

Property code	Value	Unit	Source
hf	-190.39	kJ/mol	Joback Method
hvap	71.83	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.745		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
tb	824.63	K	Joback Method
tc	1037.98	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127909493&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