

Di-t-butyl diazene N-oxide

Inchi: InChI=1S/C8H18N2O/c1-7(2,3)9-10(11)8(4,5)6/h1-6H3/b10-9-
InchiKey: YOGGJOULZPUAHF-KTKRTIGZSA-N
Formula: C8H18N2O
SMILES: CC(C)(C)N=[N+][O-]C(C)(C)C
Mol. weight [g/mol]: 158.24
CAS: 54168-23-9

Physical Properties

Property code	Value	Unit	Source
chl	-5567.00 ± 1.80	kJ/mol	NIST Webbook
hf	-107.60 ± 2.10	kJ/mol	NIST Webbook
hfl	-153.50 ± 2.10	kJ/mol	NIST Webbook
hvap	45.90 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.546		Crippen Method
mcpvol	145.110	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54168239&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

chl: Standard liquid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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

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