

2-Tetrazene, 1,1,4,4-tetrakis(1-methylethyl)-

Other names:	1,1,4,4-Tetraisopropyl-«DELTA»-2-tetrazene
Inchi:	InChI=1S/C12H28N4/c1-9(2)15(10(3)4)13-14-16(11(5)6)12(7)8/h9-12H,1-8H3
InchiKey:	ZNDMWJNPHFHXFT-UHFFFAOYSA-N
Formula:	C12H28N4
SMILES:	CC(C)N(N=NN(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]:	228.38
CAS:	13304-31-9

Physical Properties

Property code	Value	Unit	Source
hf	-129.85	kJ/mol	Joback Method
hvap	51.51	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
log10ws	-3.67		Crippen Method
logp	3.506		Crippen Method
mcvol	215.560	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
tb	646.28	K	Joback Method
tc	840.73	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13304319&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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