1,3,5-tri(tert-butyl)-2-nitrosobenzene

Other names: 2,4,6-Tri-t-butyl-nitrosobenzene
Inchi: InChI=1S/C18H29NO/c1-16(2,3)12-10-13(17(4,5)6)15(19-20)14(11-12)18(7,8)9/h10-11H
InchiKey: OSICDPWAPKXXHT-UHFFFAOYSA-N
Formula: C18H29NO
SMILES: CC(C)(C)c1cc(C(C)(C)C)c(N=O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 275.43
CAS: 24973-59-9

Physical Properties

Property code	Value	Unit	Source
chs	-11019.30 ± 3.70	kJ/mol	NIST Webbook
hf	-117.40 ± 5.40	kJ/mol	NIST Webbook
hfs	-208.40 ± 4.40	kJ/mol	NIST Webbook
hsub	91.00 ± 3.20	kJ/mol	NIST Webbook
hsub	91.00 ± 3.20	kJ/mol	NIST Webbook
hvap	65.13	kJ/mol	Joback Method
ie	8.69	eV	NIST Webbook
log10ws	-6.17		Crippen Method
logp	5.977		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
tb	706.57	K	Joback Method
tc	920.64	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=C24973599&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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