

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]:	275.44

Physical Properties

Property code	Value	Unit	Source
hf	-120.85	kJ/mol	Cheméo Relay (1.0)
hsub	91.00 ± 3.20	kJ/mol	NIST Webbook
hsub	91.00 ± 3.20	kJ/mol	NIST Webbook
hvap	75.96	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	NIST Webbook
logp	5.977		Crippen Method
mcvol	252.270	ml/mol	McGowan Method
tb	560.99	K	Cheméo Relay (1.0)
tf	361.00	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24973599&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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