

Nitrosothymol

Other names:	2-Isopropyl-5-methyl-4-nitrosophenol p-Nitrosothymol 6-Nitrosothymol Phenol, 5-methyl-2-(1-methylethyl)-4-nitroso- Thymol, 6-nitroso- 2-Methyl-5-isopropylbenzoquinone monoxime 5-Methyl-4-nitroso-2-isopropyl phenol NSC 32670 NSC 5054
Inchi:	InChI=1S/C10H13NO2/c1-6(2)8-5-9(11-13)7(3)4-10(8)12/h4-6,12H,1-3H3
InchiKey:	YQVCMSSJMLGWAM-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	<chem>Cc1cc(O)c(C(C)C)cc1N=O</chem>
Mol. weight [g/mol]:	179.22
CAS:	2364-54-7

Physical Properties

Property code	Value	Unit	Source
hf	-386.92	kJ/mol	Joback Method
hvap	63.18	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.222		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	608.42	K	Joback Method
tc	828.03	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=C2364547&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	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

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