5-nitroindole

Other names:	indole, 5-nitro-
Inchi:	InChI=1S/C8H6N2O2/c11-10(12)7-1-2-8-6(5-7)3-4-9-8/h1-5,9H
InchiKey:	OZFPSOBLQZPIAV-UHFFFAOYSA-N
Formula:	C8H6N2O2
SMILES:	O=[N+]([O-])c1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	162.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	1.594		Crippen Method
mcvol	112.060	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	9.42e-05	kPa	353.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	9.30e-05	kPa	353.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	9.30e-05	kPa	353.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.15e-04	kPa	355.20	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

psub	1.12e-04	kPa	355.20	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.37e-04	kPa	357.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.34e-04	kPa	357.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.31e-04	kPa	357.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.72e-04	kPa	359.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.70e-04	kPa	359.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.67e-04	kPa	359.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.00e-04	kPa	361.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.01e-04	kPa	361.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.44e-04	kPa	363.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

psub	2.36e-04	kPa	363.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.14e-04	kPa	365.16	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.04e-04	kPa	365.16	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.93e-04	kPa	365.16	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.80e-04	kPa	367.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.69e-04	kPa	367.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.54e-04	kPa	367.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	4.45e-04	kPa	369.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	4.39e-04	kPa	369.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	4.32e-04	kPa	369.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

psub	5.52e-04	kPa	371.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	5.46e-04	kPa	371.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	5.33e-04	kPa	371.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.82e-04	kPa	373.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.53e-04	kPa	373.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.31e-04	kPa	373.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	8.01e-04	kPa	375.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	7.69e-04	kPa	375.17	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline:	https://www.doi.org/10.1016/j.jct.2008.09.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure

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