

1H-Indole, 2,3-dihydro-5-nitro-

Other names:	Indoline, 5-nitro- 5-Nitro-2,3-dihydroindole 5-Nitroindoline
Inchi:	InChI=1S/C8H8N2O2/c11-10(12)7-1-2-8-6(5-7)3-4-9-8/h1-2,5,9H,3-4H2
InchiKey:	WJQWYAJTPPYORB-UHFFFAOYSA-N
Formula:	C8H8N2O2
SMILES:	O=[N+]([O-])c1ccc2c(c1)CCN2
Mol. weight [g/mol]:	164.16
CAS:	32692-19-6

Physical Properties

Property code	Value	Unit	Source
gf	301.35	kJ/mol	Joback Method
hf	125.33	kJ/mol	Joback Method
hfus	27.75	kJ/mol	Joback Method
hsub	109.80 ± 0.80	kJ/mol	NIST Webbook
hvap	60.57	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.563		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	630.88	K	Joback Method
tc	898.23	K	Joback Method
tf	502.20	K	Joback Method
vc	0.453	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.85	J/molxK	630.88	Joback Method
cpg	295.70	J/molxK	675.44	Joback Method
cpg	306.55	J/molxK	720.00	Joback Method
cpg	316.51	J/molxK	764.55	Joback Method
cpg	325.67	J/molxK	809.11	Joback Method

cpg	334.11	J/mol×K	853.67	Joback Method
cpg	341.94	J/mol×K	898.23	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=C32692196&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	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
tf:	Normal melting (fusion) point
vc:	Critical Volume

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