

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

Other names:	Indan, 5-nitro- «beta»-Nitroindan 5-Nitroindan 5-Nitroindane
Inchi:	InChI=1S/C9H9NO2/c11-10(12)9-5-4-7-2-1-3-8(7)6-9/h4-6H,1-3H2
InchiKey:	DLURUQQMVLLOLCP-UHFFFAOYSA-N
Formula:	C9H9NO2
SMILES:	O=[N+](O)c1ccc2c(c1)CCC2
Mol. weight [g/mol]:	163.17
CAS:	7436-07-9

Physical Properties

Property code	Value	Unit	Source
gf	222.06	kJ/mol	Joback Method
hf	66.88	kJ/mol	Joback Method
hfus	20.75	kJ/mol	Joback Method
hvap	56.04	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.083		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
rinpol	261.38		NIST Webbook
rinpol	261.00		NIST Webbook
rinpol	261.18		NIST Webbook
rinpol	251.36		NIST Webbook
rinpol	261.00		NIST Webbook
rinpol	261.55		NIST Webbook
rinpol	258.41		NIST Webbook
rinpol	261.55		NIST Webbook
rinpol	261.65		NIST Webbook
rinpol	261.38		NIST Webbook
tb	605.21	K	Joback Method
tc	864.19	K	Joback Method
tf	408.44	K	Joback Method
vc	0.471	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.12	J/molxK	605.21	Joback Method
cpg	304.94	J/molxK	648.37	Joback Method
cpg	316.68	J/molxK	691.54	Joback Method
cpg	327.44	J/molxK	734.70	Joback Method
cpg	337.32	J/molxK	777.86	Joback Method
cpg	346.44	J/molxK	821.03	Joback Method
cpg	354.89	J/molxK	864.19	Joback Method

Sources

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=C7436079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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