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

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
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/mol×K	630.88	Joback Method
cpg	295.70	J/mol×K	675.44	Joback Method
cpg	306.55	J/mol×K	720.00	Joback Method
cpg	316.51	J/mol×K	764.55	Joback Method
cpg	325.67	J/mol×K	809.11	Joback Method
cpg	334.11	J/mol×K	853.67	Joback Method
cpg	341.94	J/mol×K	898.23	Joback Method

psub	1.88e-04	kPa	348.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	6.06e-05	kPa	338.09	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	6.30e-05	kPa	338.09	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	7.74e-05	kPa	340.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	7.36e-05	kPa	340.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	7.65e-05	kPa	340.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	1.01e-04	kPa	342.20	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	9.69e-05	kPa	342.20	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	9.36e-05	kPa	342.20	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	1.21e-04	kPa	344.08	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	

psub	1.24e-04	kPa	344.08	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.18e-04	kPa	344.08	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.52e-04	kPa	346.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.45e-04	kPa	346.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.43e-04	kPa	346.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.24e-05	kPa	338.09	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.78e-04	kPa	348.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	1.80e-04	kPa	348.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.41e-04	kPa	350.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	2.36e-04	kPa	350.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

psub	2.31e-04	kPa	350.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	2.96e-04	kPa	352.13	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	2.91e-04	kPa	352.13	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	2.79e-04	kPa	352.13	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	3.74e-04	kPa	354.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	3.44e-04	kPa	354.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	6.16e-04	kPa	360.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	4.19e-04	kPa	356.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	4.19e-04	kPa	356.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	
psub	4.13e-04	kPa	356.10	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline	

psub	5.20e-04	kPa	358.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	5.15e-04	kPa	358.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	5.00e-04	kPa	358.12	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.68e-04	kPa	360.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	6.26e-04	kPa	360.18	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
psub	3.47e-04	kPa	354.19	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline
rhos	1390.00	kg/m3	298.15	Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
psub:	Sublimation pressure
rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume