Naphthalene, 1-nitro-

Other names:	1-Nitronaftalen
	1-Nitronaphthalene
	1-Nitronapthalene
	NCI-C01956
	Nitrol
	Nitrol (pesticide)
	«alpha»-Nitronaphthalene
	Â«alphaÂ»-Nitronaphthalene
Inchi:	InChI=1S/C10H7NO2/c12-11(13)10-7-3-5-8-4-1-2-6-9(8)10/h1-7H
InchiKey:	RJKGJBPXVHTNJL-UHFFFAOYSA-N
Formula:	C10H7NO2
SMILES:	O=[N+]([O-])c1cccc2ccccc12
Mol. weight [g/mol]:	173.17
CAS:	86-57-7

Physical Properties

Property code	Value	Unit	Source
chs	-4981.26	kJ/mol	NIST Webbook
chs	-4978.50	kJ/mol	NIST Webbook
ea	1.23 ± 0.10	eV	NIST Webbook
ea	1.24 ± 0.05	eV	NIST Webbook
gf	278.30	kJ/mol	Joback Method
hf	155.64	kJ/mol	Joback Method
hfs	45.73	kJ/mol	NIST Webbook
hfus	23.69	kJ/mol	Joback Method
hsub	95.10 ± 0.40	kJ/mol	NIST Webbook
hvap	59.02	kJ/mol	Joback Method
ie	8.59	eV	NIST Webbook
ie	8.60 ± 0.01	eV	NIST Webbook
log10ws	-3.59		Aqueous Solubility Prediction Method
log10ws	-3.54		Estimated Solubility Method
logp	2.748		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	1586.00		NIST Webbook

rinpol	1589.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	274.40		NIST Webbook
rinpol	1612.87		NIST Webbook
rinpol	266.70		NIST Webbook
rinpol	1610.84		NIST Webbook
rinpol	272.40		NIST Webbook
rinpol	274.95		NIST Webbook
rinpol	273.00		NIST Webbook
rinpol	274.00		NIST Webbook
rinpol	1615.66		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	273.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1615.84		NIST Webbook
rinpol	274.07		NIST Webbook
rinpol	1615.66		NIST Webbook
rinpol	274.18		NIST Webbook
tb	577.20	K	NIST Webbook
tc	898.12	K	Joback Method
tf	330.00 ± 1.00	K	NIST Webbook
tf	329.39 ± 3.00	K	NIST Webbook
tf	327.70 ± 0.40	K	NIST Webbook
tf	332.98	K	Aqueous Solubility Prediction Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.89	J/mol×K	898.12	Joback Method
cpg	308.94	J/mol×K	675.25	Joback Method
cpg	319.67	J/mol×K	719.83	Joback Method
cpg	329.43	J/mol×K	764.40	Joback Method
cpg	338.30	J/mol×K	808.97	Joback Method
cpg	346.42	J/mol×K	853.54	Joback Method
cpg	297.11	J/mol×K	630.68	Joback Method
hfust	17.30	kJ/mol	328.90	NIST Webbook
hfust	18.43	kJ/mol	329.90	NIST Webbook

hfust	18.43	kJ/mol	329.90	NIST Webbook
hsubt	94.40 ± 0.40	kJ/mol	313.00	NIST Webbook
hsubt	68.50 ± 1.90	kJ/mol	283.00	NIST Webbook
hsubt	106.90	kJ/mol	328.50	NIST Webbook
hvapt	66.40	kJ/mol	456.00	NIST Webbook
psub	5.72e-04	kPa	315.13	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.53e-04	kPa	311.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.63e-04	kPa	313.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.57e-04	kPa	313.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	4.53e-04	kPa	313.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	5.80e-04	kPa	315.13	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.56e-04	kPa	311.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	5.74e-04	kPa	315.13	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	6.97e-04	kPa	317.13	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	7.02e-04	kPa	317.13	Thermochemistry of nitronaphthalenes and nitroanthracenes

psub	6.95e-04	kPa	317.13	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	8.75e-04	kPa	319.17	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	8.96e-04	kPa	319.17	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	8.80e-04	kPa	319.17	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.13e-03	kPa	321.14	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.11e-03	kPa	321.14	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.11e-03	kPa	321.14	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	3.52e-04	kPa	311.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.78e-04	kPa	309.16	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.82e-04	kPa	309.16	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.81e-04	kPa	309.16	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.18e-04	kPa	307.15	Thermochemistry of nitronaphthalenes and nitroanthracenes

psub	2.21e-04	kPa	307.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	2.25e-04	kPa	307.15	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.74e-04	kPa	305.14	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.73e-04	kPa	305.14	Thermochemistry of nitronaphthalenes and nitroanthracenes
psub	1.74e-04	kPa	305.14	Thermochemistry of nitronaphthalenes and nitroanthracenes

Sources

Thermochemistry of nitronaphthalenes and nitroanthracenes:	https://www.doi.org/10.1016/j.jct.2005.08.007
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume