Naphthalene, 2-nitro-

Other names:	2-Nitronaphthalene
	«beta»-Nitronaphthalene
	Â«betaÂ»-Nitronaphthalene
Inchi:	InChI=1S/C10H7NO2/c12-11(13)10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey:	ZJYJZEAJZXVAMF-UHFFFAOYSA-N
Formula:	C10H7NO2
SMILES:	O=[N+]([O-])c1ccc2ccccc2c1
Mol. weight [g/mol]:	173.17
CAS:	581-89-5

Physical Properties

Property code	Value	Unit	Source
ea	1.24 ± 0.05	eV	NIST Webbook
ea	1.18 ± 0.10	eV	NIST Webbook
gf	278.30	kJ/mol	Joback Method
hf	155.64	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	59.02	kJ/mol	Joback Method
ie	8.67 ± 0.01	eV	NIST Webbook
ie	8.63	eV	NIST Webbook
log10ws	-3.82		Aqueous Solubility Prediction Method
logp	2.748		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	280.06		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	279.20		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	280.32		NIST Webbook
rinpol	275.21		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	278.91		NIST Webbook

rinpol	280.63		NIST Webbook
rinpol	279.20		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	280.32		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	630.68	K	Joback Method
tc	898.12	K	Joback Method
tf	417.71	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.11	J/mol×K	630.68	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	353.89	J/mol×K	898.12	Joback Method
hfust	14.50	kJ/mol	348.20	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C581895&Units=SI

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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