Naphthalene, 2-methyl-1-nitro-

Other names: 1-Nitro-2-methylnaphthalene
2-Methyl-1-nitronaphthalene
Inchi: InChI=1S/C11H9NO2/c1-8-6-7-9-4-2-3-5-10(9)11(8)12(13)14/h2-7H,1H3
InchiKey: IZNWACYOILBFEG-UHFFFAOYSA-N
Formula: C11H9NO2
SMILES: Cc1ccc2ccccc2c1[N+](=O)[O-]
Mol. weight [g/mol]: 187.19
CAS: 881-03-8

Physical Properties

Property code	Value	Unit	Source
ea	1.03 ± 0.10	eV	NIST Webbook
gf	277.09	kJ/mol	Joback Method
hf	123.53	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	61.91	kJ/mol	Joback Method
log10ws	-4.27		Aqueous Solubility Prediction Method
logp	3.056		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	278.45		NIST Webbook
rinpol	275.80		NIST Webbook
rinpol	276.89		NIST Webbook
rinpol	278.52		NIST Webbook
rinpol	278.74		NIST Webbook
rinpol	272.09		NIST Webbook
rinpol	278.74		NIST Webbook
tb	658.54	K	Joback Method
tc	920.40	K	Joback Method
tf	354.65	K	Aqueous Solubility Prediction Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.19	J/mol×K	658.54	Joback Method
cpg	355.61	J/mol×K	702.18	Joback Method
cpg	366.99	J/mol×K	745.83	Joback Method
cpg	377.43	J/mol×K	789.47	Joback Method
cpg	387.03	J/mol×K	833.11	Joback Method
cpg	395.87	J/mol×K	876.76	Joback Method
cpg	404.07	J/mol×K	920.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.70	K	2.40	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=C881038&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume