4-NITRO-1-NAPHTHYLAMINE

Other names: 4-Nitro-«alpha»-naphthylamine
1-Naphthylamine, 4-nitro-
1-Amino-4-nitronaphthalene
1,4-Nitronaphthylamine
4-Nitro-1-naphthamine
4-Nitro-1-naphthylamine
4-Nitro-1-naphthalenamine
NSC 614

Inchi: InChI=1S/C10H8N2O2/c11-9-5-6-10(12(13)14)8-4-2-1-3-7(8)9/h1-6H,11H2

InchiKey: BVPJPRYNQHAOPQ-UHFFFAOYSA-N

Formula: C10H8N2O2

SMILES: Nc1ccc([N+](=O)[O-])c2ccccc12

Mol. weight [g/mol]: 188.19

Physical Properties

Property code	Value	Unit	Source
hf	121.77	kJ/mol	Cheméo Relay (1.0)
hfus	28.50	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Cheméo Relay (1.0)
ie	7.73 ± 0.02	eV	NIST Webbook
log10ws	-3.41		Cheméo Relay (1.0)
logp	2.330		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	368.60		NIST Webbook
rinpol	368.60		NIST Webbook
tb	629.28	K	Cheméo Relay (1.0)
tf	413.04	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.38	J/mol×K	708.19	Joback Method
cpg	357.24	J/mol×K	753.66	Joback Method
cpg	367.13	J/mol×K	799.14	Joback Method

cpg	376.16	J/mol×K	844.61	Joback Method
cpg	384.44	J/mol×K	890.09	Joback Method
cpg	392.09	J/mol×K	935.56	Joback Method
cpg	399.21	J/mol×K	981.03	Joback Method

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C776341&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point