

1-Naphthalenamine, 4-nitro-

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:	<chem>Nc1ccc([N+](=O)[O-])c2ccccc12</chem>
Mol. weight [g/mol]:	188.18
CAS:	776-34-1

Physical Properties

Property code	Value	Unit	Source
gf	335.12	kJ/mol	Joback Method
hf	177.96	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
ie	7.73 ± 0.02	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	2.330		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	368.60		NIST Webbook
rinpol	368.60		NIST Webbook
tb	708.19	K	Joback Method
tc	981.03	K	Joback Method
tf	513.49	K	Joback Method
vc	0.520	m3/kmol	Joback Method

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C776341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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