

# Naphthalene, 1,5-dinitro-

<b>Other names:</b>	1,5-Dinitronaphthalene
<b>Inchi:</b>	InChI=1S/C10H6N2O4/c13-11(14)9-5-1-3-7-8(9)4-2-6-10(7)12(15)16/h1-6H
<b>InchiKey:</b>	ZUTCJXFCHHDFJS-UHFFFAOYSA-N
<b>Formula:</b>	C10H6N2O4
<b>SMILES:</b>	O=[N+]([O-])c1cccc2c([N+](=O)[O-])cccc12
<b>Mol. weight [g/mol]:</b>	218.17
<b>CAS:</b>	605-71-0

## Physical Properties

Property code	Value	Unit	Source
chs	-4826.20 ± 7.10	kJ/mol	NIST Webbook
chs	-4820.40 ± 5.00	kJ/mol	NIST Webbook
chs	-4831.01	kJ/mol	NIST Webbook
ea	1.77 ± 0.10	eV	NIST Webbook
ea	2.25 ± 0.05	eV	NIST Webbook
gf	304.22	kJ/mol	Joback Method
hf	133.41	kJ/mol	Joback Method
hfs	38.40	kJ/mol	NIST Webbook
hfs	33.60 ± 7.10	kJ/mol	NIST Webbook
hfus	34.66	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	2.656		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
rinpol	325.70		NIST Webbook
rinpol	328.13		NIST Webbook
rinpol	325.70		NIST Webbook
rinpol	328.45		NIST Webbook
rinpol	328.45		NIST Webbook
tb	787.50	K	Joback Method
tc	1073.68	K	Joback Method
tf	573.84	K	Joback Method
vc	0.574	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.93	J/mol×K	1025.98	Joback Method
cpg	375.77	J/mol×K	787.50	Joback Method
cpg	385.35	J/mol×K	835.20	Joback Method
cpg	394.02	J/mol×K	882.89	Joback Method
cpg	401.92	J/mol×K	930.59	Joback Method
cpg	409.18	J/mol×K	978.29	Joback Method
cpg	422.31	J/mol×K	1073.68	Joback Method
cps	259.40	J/mol×K	323.00	NIST Webbook
hvapt	74.70	kJ/mol	574.00	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C605710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C605710&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>ea:</b>	Electron affinity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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