

Naphthalene, 1,4-dinitro-

Other names:	1,4-Dinitronaphthalene
Inchi:	InChI=1S/C10H6N2O4/c13-11(14)9-5-6-10(12(15)16)8-4-2-1-3-7(8)9/h1-6H
InchiKey:	GQBQDMFMXUHAU-UHFFFAOYSA-N
Formula:	C10H6N2O4
SMILES:	O=[N+]([O-])c1ccc([N+](=O)[O-])c2ccccc12
Mol. weight [g/mol]:	218.17
CAS:	6921-26-2

Physical Properties

Property code	Value	Unit	Source
gf	304.22	kJ/mol	Joback Method
hf	133.41	kJ/mol	Joback Method
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	320.88		NIST Webbook
tb	787.50	K	Joback Method
tc	1073.68	K	Joback Method
tf	573.84	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.77	J/molxK	787.50	Joback Method
cpg	385.35	J/molxK	835.20	Joback Method
cpg	394.02	J/molxK	882.89	Joback Method
cpg	401.92	J/molxK	930.59	Joback Method
cpg	409.18	J/molxK	978.29	Joback Method
cpg	415.93	J/molxK	1025.98	Joback Method
cpg	422.31	J/molxK	1073.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C6921262&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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