

Benzenamine, 2,4-dinitro-

Other names:	1-amino-2,4-dinitrobenzene 2,4-Dinitraniline 2,4-Dinitroanilin 2,4-Dinitroanilina 2,4-dinitroaniline 2,4-dinitrobenzenamine NCI-C60753 NSC 8731 aniline, 2,4-dinitro-
Inchi:	InChI=1S/C6H5N3O4/c7-5-2-1-4(8(10)11)3-6(5)9(12)13/h1-3H,7H2
InchiKey:	LXQOQPGNCGEELI-UHFFFAOYSA-N
Formula:	C6H5N3O4
SMILES:	Nc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	183.12
CAS:	97-02-9

Physical Properties

Property code	Value	Unit	Source
chs	-3007.71	kJ/mol	NIST Webbook
chs	-3009.40	kJ/mol	NIST Webbook
chs	-3005.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3010.00	kJ/mol	NIST Webbook
gf	230.34	kJ/mol	Joback Method
hf	58.69	kJ/mol	Joback Method
hfs	-67.95	kJ/mol	NIST Webbook
hfs	-70.30 ± 3.00	kJ/mol	NIST Webbook
hfs	-65.70	kJ/mol	NIST Webbook
hfs	-66.27	kJ/mol	NIST Webbook
hfus	32.48	kJ/mol	Joback Method
hvap	76.37	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.085		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	749.53	K	Joback Method
tc	1034.10	K	Joback Method
tf	453.05 ± 0.30	K	NIST Webbook

tf

451.20

K

Solubility determination
and thermodynamic
modeling of
2,4-dinitroaniline in nine
organic solvents from T =
(278.15 to 318.15) K and
mixing properties of
solutions

vc

0.457

m3/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.44	J/mol×K	749.53	Joback Method
cpg	306.66	J/mol×K	796.96	Joback Method
cpg	314.01	J/mol×K	844.39	Joback Method
cpg	320.54	J/mol×K	891.81	Joback Method
cpg	326.32	J/mol×K	939.24	Joback Method
cpg	331.39	J/mol×K	986.67	Joback Method
cpg	335.82	J/mol×K	1034.10	Joback Method

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C97029&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Solubility determination and
thermodynamic modeling of

2,4-dinitroaniline in nine organic
solvents from T = (278.15 to 318.15) K
and mixing properties of solutions:

<https://www.doi.org/10.1016/j.jct.2016.07.009>
https://en.wikipedia.org/wiki/Joback_method
<http://link.springer.com/article/10.1007/BF02311772>

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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