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

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
hf	81.74	kJ/mol	Cheméo Relay (1.0)
hfs	-70.30 ± 3.00	kJ/mol	NIST Webbook
hfs	-66.27	kJ/mol	NIST Webbook
hfs	-67.95	kJ/mol	NIST Webbook
hfs	-65.70	kJ/mol	NIST Webbook
hfus	32.48	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	-2.69		Cheméo Relay (1.0)
logp	1.085		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
tb	571.00	K	Cheméo Relay (1.0)
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

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97029&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point