

Benzoic acid, 3,5-dinitro-

Other names:	2,4-dinitrobenzoic acid 3,5-Dinitrobenzoic acid 3-Carboxy-1,5-Dinitrobenzene DNBA Dinitrobenzoic acid benzoic acid, 2,4-dinitro-
Inchi:	InChI=1S/C7H4N2O6/c10-7(11)4-1-5(8(12)13)3-6(2-4)9(14)15/h1-3H,(H,10,11)
InchiKey:	VYWYYJYRVSBHJQ-UHFFFAOYSA-N
Formula:	C7H4N2O6
SMILES:	O=C(O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	212.12
CAS:	99-34-3

Physical Properties

Property code	Value	Unit	Source
chs	-2894.00 ± 0.40	kJ/mol	NIST Webbook
gf	-93.43	kJ/mol	Joback Method
hf	-260.55	kJ/mol	Joback Method
hfs	-432.60 ± 0.40	kJ/mol	NIST Webbook
hfus	30.60	kJ/mol	Vapor pressures and standard molar enthalpies, entropies, and Gibbs free energies of sublimation of 2,4- and 3,4-dinitrobenzoic acids
hvap	91.38	kJ/mol	Joback Method
log10ws	-2.42		Aqueous Solubility Prediction Method
logp	1.201		Crippen Method
mcvol	128.010	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
tb	845.93	K	Joback Method
tc	1098.09	K	Joback Method
tf	478.82	K	Aqueous Solubility Prediction Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.32	J/mol×K	845.93	Joback Method
cpg	343.27	J/mol×K	887.96	Joback Method
cpg	348.56	J/mol×K	929.98	Joback Method
cpg	353.23	J/mol×K	972.01	Joback Method
cpg	357.31	J/mol×K	1014.04	Joback Method
cpg	360.85	J/mol×K	1056.06	Joback Method
cpg	363.88	J/mol×K	1098.09	Joback Method
hfust	22.80	kJ/mol	480.40	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C99343&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Determination and modeling of binary and ternary solid-liquid phase equilibria for the systems formed by <https://www.doi.org/10.1016/j.jct.2016.10.004>

Solubility of 3,5-Dinitrobenzoic Acid in Supercritical Carbon Dioxide with <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Vapor pressures and standard molar <https://www.doi.org/10.1021/je100331h>

enthalpies, entropies, and Gibbs free <https://www.doi.org/10.1016/j.jct.2009.02.008>

energies of sublimation of 2,4 and <https://www.doi.org/10.1016/j.tca.2011.01.039>

3,5-dinitrobenzoic acid and https://en.wikipedia.org/wiki/Joback_method

3-nitrobenzoic acid in supercritical carbon dioxide:

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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