Benzene, 1,2-dinitro-

Other names:	1,2-Dinitrobenzene
	1,2-Dinitrobenzol
	Benzene, o-dinitro-
	UN 1597
	o-Dinitrobenzene
	ortho-Dinitrobenzene
Inchi:	InChI=1S/C6H4N2O4/c9-7(10)5-3-1-2-4-6(5)8(11)12/h1-4H
InchiKey:	IZUKQUVSCNEFMJ-UHFFFAOYSA-N
Formula:	C6H4N2O4
SMILES:	O=[N+]([O-])c1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	168.11
CAS:	528-29-0

Physical Properties

Property code	Value	Unit	Source
chs	-2931.00 ± 0.63	kJ/mol	NIST Webbook
chs	-2945.00	kJ/mol	NIST Webbook
ea	1.77 ± 0.05	eV	NIST Webbook
ea	1.65 ± 0.10	eV	NIST Webbook
gf	173.52	kJ/mol	Joback Method
hf	36.37	kJ/mol	Joback Method
hfs	-2.00 ± 0.63	kJ/mol	NIST Webbook
hfus	27.67	kJ/mol	Joback Method
hsub	87.90 ± 2.10	kJ/mol	NIST Webbook
hsub	95.50 ± 0.90	kJ/mol	NIST Webbook
hvap	65.07	kJ/mol	Joback Method
ie	10.71	eV	NIST Webbook
log10ws	-3.10		Aqueous Solubility Prediction Method
log10ws	-3.10		Estimated Solubility Method
logp	1.503		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=4)		KDB
pc	4730.11	kPa	Joback Method

tb	672.02	K	Joback Method
tc	952.61	K	Joback Method
tf	390.10 ± 0.20	K	NIST Webbook
tf	391.40	K	Aqueous Solubility Prediction Method
tf	387.70 ± 0.10	K	NIST Webbook
tf	390.00 ± 2.00	K	NIST Webbook
tf	390.05 ± 0.20	K	NIST Webbook
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.14	J/mol×K	672.02	Joback Method
cpg	271.07	J/mol×K	765.55	Joback Method
cpg	278.24	J/mol×K	812.32	Joback Method
cpg	284.63	J/mol×K	859.08	Joback Method
cpg	290.30	J/mol×K	905.85	Joback Method
cpg	295.30	J/mol×K	952.61	Joback Method
cpg	263.06	J/mol×K	718.79	Joback Method
cps	195.00	J/mol×K	298.00	NIST Webbook
cps	186.20	J/mol×K	297.90	NIST Webbook
cps	200.40	J/mol×K	298.15	NIST Webbook
hfust	22.84	kJ/mol	396.10	NIST Webbook
hfust	22.84	kJ/mol	396.10	NIST Webbook
hfust	22.75	kJ/mol	390.05	NIST Webbook
hfust	22.84	kJ/mol	396.10	NIST Webbook
hsubt	93.10 ± 0.90	kJ/mol	338.00	NIST Webbook
hsubt	82.90	kJ/mol	365.00	NIST Webbook
hsubt	87.00 ± 1.00	kJ/mol	333.00	NIST Webbook
hsubt	86.60 ± 1.20	kJ/mol	333.00	NIST Webbook
hvapt	60.00	kJ/mol	523.50	NIST Webbook
psub	3.42e-04	kPa	323.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range

psub	1.06e-03	kPa	333.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	2.92e-03	kPa	343.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	1.08e-04	kPa	313.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	7.42e-03	kPa	353.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.02	kPa	363.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
psub	0.08	kPa	383.15	Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range
sfust	58.30	J/mol×K	390.05	NIST Webbook
sfust	58.60	J/mol×K	396.10	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	592.20	K	103.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56327e+01
Coeff. B	-5.35249e+03
Coeff. C	-1.06246e+02
Temperature range (K), min.	455.05
Temperature range (K), max.	624.84

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.29655e+02
Coeff. B	-1.55190e+04
Coeff. C	-1.57127e+01
Coeff. D	4.18666e-06
Temperature range (K), min.	390.08
Temperature range (K), max.	831.00

Sources

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1437

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1437

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C528290&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Triacetone triperoxide thermogravimetric study of vapor pressure and enthalpy of sublimation in 303 338 K temperature range:	https://www.doi.org/10.1016/j.tca.2010.11.034

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume