Phenol, 2,4-dinitro-

Other names:	1-Hydroxy-2,4-dinitrobenzene
	2,4-DINITROPHENOL
	2,4-DNP
	2,4-Dinitrofenol
	ALPHA-DINITROPHENOL
	Aldifen
	Chemox PE
	DNP
	Dinitrofenolo
	Dinitrophenol
	Dinofan
	EK 102
	Fenoxyl Carbon N
	Maroxol-50
	NITROPHENE
	NSC 1532
	Nitro kleenup
	Nitrophen
	Phenol, «alpha»-dinitro-
	Phenol, Â«alphaÂ»-dinitro-
	Rcra waste number P048
	Solfo Black 2B Supra
	Solfo Black B
	Solfo Black BB
	Solfo Black G
	Solfo Black SB
	Tertrosulfur PBR
	Tertrosulfur black pb
	Tertrosulphur Black PB
	Tertrosulphur PBR
	X 32
	«alpha»-Dinitrophenol
	Â«alphaÂ»-Dinitrophenol
Inchi:	InChI=1S/C6H4N2O5/c9-6-2-1-4(7(10)11)3-5(6)8(12)13/h1-3,9H
InchiKey:	UFBJCMHMOXMLKC-UHFFFAOYSA-N
Formula:	C6H4N2O5
SMILES:	O=[N+]([O-])c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	184.11
CAS:	51-28-5

Physical Properties

Property code	Value	Unit	Source
chs	-2720.00	kJ/mol	NIST Webbook
chs	-2697.20 ± 3.20	kJ/mol	NIST Webbook
chs	-2696.90 ± 2.70	kJ/mol	NIST Webbook
chs	-2703.10 ± 2.70	kJ/mol	NIST Webbook
chs	-2709.68	kJ/mol	NIST Webbook
gf	18.90	kJ/mol	Joback Method
hf	-140.94	kJ/mol	Joback Method
hfs	-223.00	kJ/mol	NIST Webbook
hfs	-235.50	kJ/mol	NIST Webbook
hfus	33.45	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
ie	9.57	eV	NIST Webbook
log10ws	-2.32		Crippen Method
logp	1.209		Crippen Method
mcvol	112.350	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	257.00		NIST Webbook
rinpol	258.24		NIST Webbook
rinpol	257.00		NIST Webbook
tb	752.64	K	Joback Method
tc	1038.65	K	Joback Method
tf	388.00 ± 0.20	K	NIST Webbook
tf	385.95	K	KDB
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.02	J/mol×K	990.98	Joback Method
cpg	287.91	J/mol×K	752.64	Joback Method
cpg	295.32	J/mol×K	800.31	Joback Method
cpg	302.18	J/mol×K	847.98	Joback Method

cpg	308.65	J/mol×K	895.64	Joback Method
cpg	314.88	J/mol×K	943.31	Joback Method
cpg	327.23	J/mol×K	1038.65	Joback Method
hfust	24.17	kJ/mol	388.00	NIST Webbook
hfust	24.17	kJ/mol	388.00	NIST Webbook
hfust	26.19	kJ/mol	383.20	NIST Webbook
hfust	24.17	kJ/mol	388.00	NIST Webbook
hsubt	104.60 ± 4.20	kJ/mol	293.00	NIST Webbook
hsubt	104.60 ± 4.20	kJ/mol	313.00	NIST Webbook
sfust	62.30	J/mol×K	388.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.00816e+01
Coeff. B	-1.25851e+04
Coeff. C	3.92271e-03
Coeff. D	-6.67004e-09
Temperature range (K), min.	293.15
Temperature range (K), max.	333.15

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51285&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1440

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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1440

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
hsubt:	Enthalpy of sublimation at a given temperature
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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume