Phenol, 2,6-dinitro-

Other names:	o-Dinitrophenol
	Phenol, «beta»-dinitro-
	2,6-Dinitrophenol
	«beta»-Dinitrophenol
	2,6-Dinitrofenol
	Dinitro-2,6-phenol
Inchi:	InChI=1S/C6H4N2O5/c9-6-4(7(10)11)2-1-3-5(6)8(12)13/h1-3,9H
InchiKey:	JCRIDWXIBSEOEG-UHFFFAOYSA-N
Formula:	C6H4N2O5
SMILES:	O=[N+]([O-])c1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	184.11
CAS:	573-56-8

Physical Properties

Property code	Value	Unit	Source
chs	-2722.80 ± 2.70	kJ/mol	NIST Webbook
chs	-2723.10 ± 3.20	kJ/mol	NIST Webbook
gf	18.90	kJ/mol	Joback Method
hf	-140.94	kJ/mol	Joback Method
hfs	-209.60 ± 3.30	kJ/mol	NIST Webbook
hfus	33.45	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.209		Crippen Method
mcvol	112.350	ml/mol	McGowan Method
pc	5871.90	kPa	Joback Method
tb	752.64	K	Joback Method
tc	1038.65	K	Joback Method
tf	385.00 ± 3.00	K	NIST Webbook
tf	336.00 ± 0.20	K	NIST Webbook
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	19.58	kJ/mol	336.00	NIST Webbook
hfust	19.58	kJ/mol	336.00	NIST Webbook
hfust	22.91	kJ/mol	329.00	NIST Webbook
hfust	19.58	kJ/mol	336.00	NIST Webbook
hsubt	112.10 ± 4.20	kJ/mol	293.00	NIST Webbook
hsubt	112.10 ± 4.20	kJ/mol	313.00	NIST Webbook
sfust	58.26	J/mol×K	336.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C573568&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume