

Phenol, 4-methyl-2,6-dinitro-

Other names:	p-Cresol, 2,6-dinitro- 2,6-Dinitro-p-cresol 2,6-Dinitro-4-methylphenol 4-Methyl-2,6-dinitrophenol Dinitro-p-cresol DNPC Victoria Orange Victoria Yellow 2,6-Dinitro-4-cresol NSC 33870
Inchi:	InChI=1S/C7H6N2O5/c1-4-2-5(8(11)12)7(10)6(3-4)9(13)14/h2-3,10H,1H3
InchiKey:	HOYRZHJJAHMMLL-UHFFFAOYSA-N
Formula:	C7H6N2O5
SMILES:	Cc1cc([N+](=O)[O-])c(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	198.13
CAS:	609-93-8

Physical Properties

Property code	Value	Unit	Source
chs	-3372.80	kJ/mol	NIST Webbook
gf	17.69	kJ/mol	Joback Method
hf	-173.05	kJ/mol	Joback Method
hfs	-239.00	kJ/mol	NIST Webbook
hfus	35.65	kJ/mol	Joback Method
hvap	80.97	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	1.517		Crippen Method
mcvol	126.440	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
tb	780.50	K	Joback Method
tc	1059.76	K	Joback Method
tf	619.05	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.95	J/mol×K	780.50	Joback Method
cpg	343.28	J/mol×K	827.04	Joback Method
cpg	351.09	J/mol×K	873.59	Joback Method
cpg	358.52	J/mol×K	920.13	Joback Method
cpg	365.69	J/mol×K	966.67	Joback Method
cpg	372.74	J/mol×K	1013.21	Joback Method
cpg	379.80	J/mol×K	1059.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609938&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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