Phenol, 2,5-dinitro-

Other names: Phenol, «gamma»-dinitro-
2,5-Dinitrophenol
2,5-Dnp
«gamma»-Dinitrophenol
2,5-Dinitrofenol
Inchi: InChI=1S/C6H4N2O5/c9-6-3-4(7(10)11)1-2-5(6)8(12)13/h1-3,9H
InchiKey: UWEZBKLLMKVIPI-UHFFFAOYSA-N
Formula: C6H4N2O5
SMILES: O=[N+]([O-])c1ccc([N+](=O)[O-])c(O)c1
Mol. weight [g/mol]: 184.11
CAS: 329-71-5

Physical Properties

Property code	Value	Unit	Source
gf	18.90	kJ/mol	Joback Method
hf	-140.94	kJ/mol	Joback Method
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	381.00 ± 0.20	K	NIST Webbook
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	321.02	J/mol×K	990.98	Joback Method
cpg	287.91	J/mol×K	752.64	Joback Method
cpg	327.23	J/mol×K	1038.65	Joback Method
hfust	23.73	kJ/mol	381.00	NIST Webbook
hfust	23.73	kJ/mol	381.00	NIST Webbook
hfust	23.73	kJ/mol	381.00	NIST Webbook
hsubt	93.40	kJ/mol	305.50	NIST Webbook
sfust	62.28	J/mol×K	381.00	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=C329715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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