Phenol, 2,3,4,6-tetranitro

Inchi: InChI=1S/C6H2N4O9/c11-6-3(8(14)15)1-2(7(12)13)4(9(16)17)5(6)10(18)19/h1,11H
InchiKey: PXPBDJVBNWDUFM-UHFFFAOYSA-N
Formula: C6H2N4O9
SMILES: O=[N+]([O-])c1cc([N+](=O)[O-])c([N+](=O)[O-])c([N+](=O)[O-])c1O
Mol. weight [g/mol]: 274.10
CAS: 641-16-7

Physical Properties

Property code	Value	Unit	Source
gf	70.74	kJ/mol	Joback Method
hf	-185.40	kJ/mol	Joback Method
hfus	55.40	kJ/mol	Joback Method
hvap	112.59	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	1.025		Crippen Method
mcvol	147.190	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
tb	1066.28	K	Joback Method
tc	1375.51	K	Joback Method
tf	907.52	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.31	J/mol×K	1066.28	Joback Method
cpg	424.16	J/mol×K	1117.82	Joback Method
cpg	431.25	J/mol×K	1169.36	Joback Method
cpg	438.77	J/mol×K	1220.89	Joback Method
cpg	446.90	J/mol×K	1272.43	Joback Method
cpg	455.83	J/mol×K	1323.97	Joback Method
cpg	465.74	J/mol×K	1375.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C641167&Units=SI

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
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