Phenol, 2-(1,1-dimethylethyl)-4,6-dinitro-

Other names:	2,4-Dinitro-6-tert-butylphenol
	2-(1,1-Dimethylethyl)-4,6-dinitrophenol
	2-tert-Butyl-4,6-dinitrophenol
	4,6-Dinitro-2-tert-butylphenol
	Dinoterbe
	Dntbp
	Herbogil
	NSC 166496
	Phenol, 2-(1,1-dimethylethyl)-4,6-dinitro-
	Phenol, 2-t-butyl-4,6-dinitro-
	Phenol, 2-tert-butyl-4,6-dinitro-
	Phenol, o-t-butyl-4,6-dinitro-
	Phenol, o-tert-butyl-4,6-dinitro-
	Stirpan forte
Inchi:	InChI=1S/C10H12N2O5/c1-10(2,3)7-4-6(11(14)15)5-8(9(7)13)12(16)17/h4-5,13H,1-3H3
InchiKey:	IIPZYDQGBIWLBU-UHFFFAOYSA-N
Formula:	C10H12N2O5
SMILES:	CC(C)(C)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1O
Mol. weight [g/mol]:	240.22

Physical Properties

Property code	Value	Unit	Source
hf	-194.14	kJ/mol	Cheméo Relay (1.0)
hfus	36.01	kJ/mol	Joback Method
hvap	85.21	kJ/mol	Cheméo Relay (1.0)
ie	9.08	eV	Cheméo Relay (1.0)
log10ws	-3.79		Cheméo Relay (1.0)
logp	2.506		Crippen Method
mcvol	168.710	ml/mol	McGowan Method
tb	542.82	K	Cheméo Relay (1.0)
tf	382.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.25	J/mol×K	845.91	Joback Method
cpg	503.08	J/mol×K	891.65	Joback Method
cpg	513.38	J/mol×K	937.38	Joback Method
cpg	523.35	J/mol×K	983.12	Joback Method
cpg	533.17	J/mol×K	1028.86	Joback Method
cpg	543.04	J/mol×K	1074.59	Joback Method
cpg	553.14	J/mol×K	1120.33	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1420071&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point