

Dinoterb

Other names:	Phenol, 2-(1,1-dimethylethyl)-4,6-dinitro- Phenol, 2-tert-butyl-4,6-dinitro- Dinoterbe Stirpan forte 2-tert-Butyl-4,6-dinitrophenol 2,4-Dinitro-6-tert-butylphenol Phenol, o-tert-butyl-4,6-dinitro- Phenol, o-t-butyl-4,6-dinitro- 2-(1,1-Dimethylethyl)-4,6-dinitrophenol Dntbp Herbogil Phenol, 2-t-butyl-4,6-dinitro- 4,6-Dinitro-2-tert-butylphenol NSC 166496
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]:	240.21
CAS:	1420-07-1

Physical Properties

Property code	Value	Unit	Source
gf	45.79	kJ/mol	Joback Method
hf	-243.72	kJ/mol	Joback Method
hfus	36.01	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.506		Crippen Method
mcvol	168.710	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
tb	845.91	K	Joback Method
tc	1120.33	K	Joback Method
tf	655.28	K	Joback Method
vc	0.607	m3/kmol	Joback Method

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:	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=C1420071&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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