Phenol, 2,4-di-t-butyl-6-nitro-

Inchi: InChI=1S/C14H21NO3/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(8-9)15(17)18/h7-8,16H,1-6H
InchiKey: GVKJWGRAPDVEMC-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CC(C)(C)c1cc([N+](=O)[O-])c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 251.32
CAS: 20039-94-5

Physical Properties

Property code	Value	Unit	Source
gf	46.76	kJ/mol	Joback Method
hf	-324.27	kJ/mol	Joback Method
hfus	27.60	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.895		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	782.36	K	Joback Method
tc	1032.60	K	Joback Method
tf	559.17	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.81	J/mol×K	782.36	Joback Method
cpg	632.82	J/mol×K	824.07	Joback Method
cpg	646.95	J/mol×K	865.77	Joback Method
cpg	660.38	J/mol×K	907.48	Joback Method
cpg	673.28	J/mol×K	949.19	Joback Method
cpg	685.86	J/mol×K	990.89	Joback Method
cpg	698.29	J/mol×K	1032.60	Joback Method

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=C20039945&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
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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