Phenol, 4-tert.-octyl-2-nitro

Inchi: InChI=1S/C14H21NO3/c1-13(2,3)9-14(4,5)10-6-7-12(16)11(8-10)15(17)18/h6-8,16H,9H2
InchiKey: BHSFQPGUTBZBDA-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CC(C)(C)CC(C)(C)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
gf	56.39	kJ/mol	Joback Method
hf	-312.80	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.014		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	777.38	K	Joback Method
tc	1026.89	K	Joback Method
tf	546.65	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.07	J/mol×K	777.38	Joback Method
cpg	634.16	J/mol×K	818.96	Joback Method
cpg	648.33	J/mol×K	860.55	Joback Method
cpg	661.77	J/mol×K	902.13	Joback Method
cpg	674.67	J/mol×K	943.72	Joback Method
cpg	687.23	J/mol×K	985.30	Joback Method
cpg	699.64	J/mol×K	1026.89	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=R58824&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume