4-Tert-butyl-2-nitrophenol

Other names: Phenol, 4-(1,1-dimethylethyl)-2-nitro
Inchi: InChI=1S/C10H13NO3/c1-10(2,3)7-4-5-9(12)8(6-7)11(13)14/h4-6,12H,1-3H3
InchiKey: IHGNADPMUSNTJW-UHFFFAOYSA-N
Formula: C10H13NO3
SMILES: CC(C)(C)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 195.22
CAS: 3279-07-0

Physical Properties

Property code	Value	Unit	Source
gf	19.87	kJ/mol	Joback Method
hf	-221.49	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.598		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
tb	689.09	K	Joback Method
tc	946.78	K	Joback Method
tf	499.15	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.40	J/mol×K	689.09	Joback Method
cpg	420.93	J/mol×K	732.04	Joback Method
cpg	432.51	J/mol×K	774.99	Joback Method
cpg	443.29	J/mol×K	817.94	Joback Method
cpg	453.43	J/mol×K	860.88	Joback Method
cpg	463.09	J/mol×K	903.83	Joback Method

cpg	472.43	J/mol×K	946.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3279070&Units=SI
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

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