Phenol, 2-(1,1-dimethylpropyl)-4-nitro

Inchi: InChI=1S/C11H15NO3/c1-4-11(2,3)9-7-8(12(14)15)5-6-10(9)13/h5-7,13H,4H2,1-3H3
InchiKey: UANRRFFKYCFDKZ-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCC(C)(C)c1cc([N+](=O)[O-])ccc1O
Mol. weight [g/mol]: 209.24

Physical Properties

Property code	Value	Unit	Source
gf	28.29	kJ/mol	Joback Method
hf	-242.13	kJ/mol	Joback Method
hfus	27.63	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.988		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tb	711.97	K	Joback Method
tc	963.76	K	Joback Method
tf	510.42	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.65	J/mol×K	711.97	Joback Method
cpg	471.84	J/mol×K	753.94	Joback Method
cpg	484.09	J/mol×K	795.90	Joback Method
cpg	495.56	J/mol×K	837.87	Joback Method
cpg	506.41	J/mol×K	879.83	Joback Method
cpg	516.79	J/mol×K	921.80	Joback Method
cpg	526.84	J/mol×K	963.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R58593&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