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

Inchi: InChI=1S/C9H11NO3/c1-6(2)7-3-4-9(11)8(5-7)10(12)13/h3-6,11H,1-2H3
InchiKey: QYODOKUESLGDSA-UHFFFAOYSA-N
Formula: C9H11NO3
SMILES: CC(C)c1ccc(O)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 181.19

Physical Properties

Property code	Value	Unit	Source
gf	6.17	kJ/mol	Joback Method
hf	-197.38	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hvap	67.78	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.424		Crippen Method
mcvol	137.200	ml/mol	McGowan Method
pc	3920.94	kPa	Joback Method
rinpol	1276.00		NIST Webbook
tb	669.00	K	Joback Method
tc	922.53	K	Joback Method
tf	470.46	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.64	J/mol×K	669.00	Joback Method
cpg	368.31	J/mol×K	711.26	Joback Method
cpg	379.13	J/mol×K	753.51	Joback Method
cpg	389.22	J/mol×K	795.77	Joback Method
cpg	398.69	J/mol×K	838.02	Joback Method
cpg	407.65	J/mol×K	880.28	Joback Method
cpg	416.22	J/mol×K	922.53	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=R58806&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume