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

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

Physical Properties

Property code	Value	Unit	Source
gf	23.01	kJ/mol	Joback Method
hf	-238.66	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	72.23	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.204		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1861.00		NIST Webbook
tb	714.76	K	Joback Method
tc	957.31	K	Joback Method
tf	493.00	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.33	J/mol×K	714.76	Joback Method
cpg	469.42	J/mol×K	755.18	Joback Method
cpg	481.65	J/mol×K	795.61	Joback Method
cpg	493.15	J/mol×K	836.03	Joback Method
cpg	504.02	J/mol×K	876.46	Joback Method
cpg	514.36	J/mol×K	916.88	Joback Method
cpg	524.29	J/mol×K	957.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R58664&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

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