Phenol, 2-(1-methylpropyl)-6-nitro

Inchi: InChI=1S/C10H13NO3/c1-3-7(2)8-5-4-6-9(10(8)12)11(13)14/h4-7,12H,3H2,1-2H3
InchiKey: FPHJBQJDAVOGLD-UHFFFAOYSA-N
Formula: C10H13NO3
SMILES: CCC(C)c1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 195.22

Physical Properties

Property code	Value	Unit	Source
gf	14.59	kJ/mol	Joback Method
hf	-218.02	kJ/mol	Joback Method
hfus	28.93	kJ/mol	Joback Method
hvap	70.01	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.814		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	3488.88	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
tb	691.88	K	Joback Method
tc	939.72	K	Joback Method
tf	481.73	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.79	J/mol×K	691.88	Joback Method
cpg	418.22	J/mol×K	733.19	Joback Method
cpg	429.79	J/mol×K	774.49	Joback Method
cpg	440.63	J/mol×K	815.80	Joback Method
cpg	450.84	J/mol×K	857.11	Joback Method
cpg	460.53	J/mol×K	898.41	Joback Method
cpg	469.82	J/mol×K	939.72	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=R58749&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