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

Inchi: InChI=1S/C14H21NO3/c1-3-5-8-11(7-4-2)12-9-6-10-13(14(12)16)15(17)18/h6,9-11,16H,3
InchiKey: KRNGPGDUTOADKR-UHFFFAOYSA-N
Formula: C14H21NO3
SMILES: CCCCC(CCC)c1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 251.32

Physical Properties

Property code	Value	Unit	Source
gf	48.27	kJ/mol	Joback Method
hf	-300.58	kJ/mol	Joback Method
hfus	39.29	kJ/mol	Joback Method
hvap	78.91	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.374		Crippen Method
mcvol	207.650	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
tb	783.40	K	Joback Method
tc	1012.85	K	Joback Method
tf	526.81	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.59	J/mol×K	783.40	Joback Method
cpg	630.20	J/mol×K	821.64	Joback Method
cpg	644.00	J/mol×K	859.88	Joback Method
cpg	657.08	J/mol×K	898.13	Joback Method
cpg	669.55	J/mol×K	936.37	Joback Method
cpg	681.51	J/mol×K	974.61	Joback Method
cpg	693.07	J/mol×K	1012.85	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=R58753&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