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

Inchi: InChI=1S/C12H17NO3/c1-3-6-9(4-2)10-7-5-8-11(12(10)14)13(15)16/h5,7-9,14H,3-4,6H2
InchiKey: OXKMZSZQCOKAFN-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CCCC(CC)c1cccc([N+](=O)[O-])c1O
Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
gf	31.43	kJ/mol	Joback Method
hf	-259.30	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.594		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	1629.00		NIST Webbook
tb	737.64	K	Joback Method
tc	975.34	K	Joback Method
tf	504.27	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.19	J/mol×K	737.64	Joback Method
cpg	521.85	J/mol×K	777.26	Joback Method
cpg	534.66	J/mol×K	816.87	Joback Method
cpg	546.75	J/mol×K	856.49	Joback Method
cpg	558.20	J/mol×K	896.11	Joback Method
cpg	569.14	J/mol×K	935.72	Joback Method
cpg	579.66	J/mol×K	975.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R58628&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