p-t-amyl-nitrobenzene radical

Inchi: InChI=1S/C11H15NO2/c1-4-11(2,3)9-5-7-10(8-6-9)12(13)14/h5-8H,4H2,1-3H3
InchiKey: LLLHRFJRKDQEIY-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CCC(C)(C)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 193.24
CAS: 6284-98-6

Physical Properties

Property code	Value	Unit	Source
ea	2.17 ± 0.17	eV	NIST Webbook
gf	182.91	kJ/mol	Joback Method
hf	-64.82	kJ/mol	Joback Method
hfus	21.85	kJ/mol	Joback Method
hvap	58.31	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.282		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
tb	631.35	K	Joback Method
tc	875.64	K	Joback Method
tf	398.70	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.14	J/mol×K	631.35	Joback Method
cpg	425.51	J/mol×K	672.06	Joback Method
cpg	439.68	J/mol×K	712.78	Joback Method
cpg	452.74	J/mol×K	753.49	Joback Method
cpg	464.77	J/mol×K	794.21	Joback Method
cpg	475.86	J/mol×K	834.92	Joback Method
cpg	486.10	J/mol×K	875.64	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6284986&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume