3-Nitrobenzyl radical

Inchi: InChI=1S/C7H6NO2/c1-6-3-2-4-7(5-6)8(9)10/h2-5H,1H2
InchiKey: PRJWEPRQDKFJHV-UHFFFAOYSA-N
Formula: C7H6NO2
SMILES: [CH2]c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 136.13
CAS: 61219-63-4

Physical Properties

Property code	Value	Unit	Source
ea	1.59 ± 0.16	eV	NIST Webbook
gf	198.77	kJ/mol	Joback Method
hf	82.30	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	50.56	kJ/mol	Joback Method
ie	8.60 ± 0.10	eV	NIST Webbook
log10ws	-2.22		Crippen Method
logp	1.777		Crippen Method
mcvol	101.000	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	542.36	K	Joback Method
tc	787.99	K	Joback Method
tf	367.57	K	Joback Method
vc	0.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.02	J/mol×K	542.36	Joback Method
cpg	222.88	J/mol×K	583.30	Joback Method
cpg	231.88	J/mol×K	624.24	Joback Method
cpg	240.11	J/mol×K	665.17	Joback Method
cpg	247.66	J/mol×K	706.11	Joback Method
cpg	254.59	J/mol×K	747.05	Joback Method
cpg	261.00	J/mol×K	787.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61219634&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
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
ie:	Ionization energy
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