benzoate anion

Inchi: InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)/p-1
InchiKey: WPYMKLBDIGXBTP-UHFFFAOYSA-M
Formula: C7H5O2-
SMILES: O=C([O-])c1ccccc1
Mol. weight [g/mol]: 121.11
CAS: 766-76-7

Physical Properties

Property code	Value	Unit	Source
ean	3.59 ± 0.05	eV	NIST Webbook
ean	3.60 ± 0.10	eV	NIST Webbook
ean	3.75 ± 0.16	eV	NIST Webbook
log10ws	-4.23		Crippen Method
logp	0.050		Crippen Method
mcvol	91.020	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C766767&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ean: Electron affinity of neutral species
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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