

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/ci9903071>

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

Latest version available from:

<https://www.cheméo.com/cid/28-559-1/benzoate-anion.pdf>

Generated by Cheméo on 2024-04-26 16:56:50.925397772 +0000 UTC m=+16439859.845975085.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.