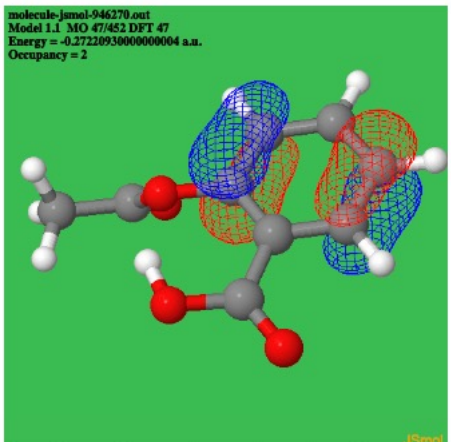
Results from an EMSL Arrows Calculation

EMSL Arrows is a revolutionary approach to materials and chemical simulations that uses NWChem and chemical computational databases to make materials and chemical modeling accessible via a broad spectrum of digital communications including posts to web APIs, social networks, and traditional email.

Molecular modeling software has previously been extremely complex, making it prohibative to all but experts in the field, yet even experts can struggle to perform calculations. This service is designed to be used by experts and non-experts alike. Experts can carry out and keep track of large numbers of complex calculations with diverse levels of theories present in their workflows. Additionally, due to a streamlined and easy-to-use input, non-experts can carry out a wide variety of molecular modeling calculations previously not accessible to them.

```
The id(s) for esmiles = CC(=O)Oc1ccccc1C(=O)O theory{dft} xc{b3lyp} basis{6-311++G(2d,2p)} solvation_type{COSMO} ^{0} are: 13290 13473 33587 34719 42925
Use id=% instead of esmiles to print other entries.

mformula      = C9H8O4
iupac         = 2-acetyloxybenzoic acid
PubChem       = 2244
PubChem LCSS  = 2244
cas           = 50-78-2
kegg          = C01405 D00109
synonyms      = aspirin; ACETYLSALICYLIC ACID; 2-Acetoxybenzoic acid; Ecotrin; 2-(Acetyloxy)benzoic acid; Acenterine; Acetosal; Acylpyrin; Polopiryna; 50-78-2; Acetophen; Aspergum; Easprin; Rh

Search Links to Other Online Resources (may not be available):
  - Google Structure Search
  - EPA CompTox Database
  - Chemical Entities of Biological Interest (ChEBI)
  - NIH ChemIDplus - A TOXNET DATABASE
  - The Human Metabolome Database (HMDB)
  - OECD eChemPortal
  - Google Scholar


  +================================================+
  ||              Molecular Calculation           ||
  +================================================+

  Id      = 33587

  NWOutput = Link to NWChem Output (download)

  Datafiles:
  lumo-restricted.cube-2016-8-3-3:59:10 (download)
  homo-restricted.cube-2016-8-3-3:59:10 (download)
  mo_orbital_nwchemarrows.out-?54304-2017-12-4-21:37:12 (download)

  image_resset: api/image_reset/33587

  Calculation performed by orbital
  Numbers of cpus used for calculation = 4
  Calculation walltime = 147398.600000 seconds (1 days 16 hours 56 minutes 38 seconds)


  +-----------------+
  | Energetic Data |
  +-----------------+

  Id        = 33587
  iupac     = 2-acetyloxybenzoic acid
  mformula  = C9H8O4
  inchi     = InChI=1S/C9H8O4/c1-6(10)13-8-5-3-2-4-7(8)9(11)12/h2-5H,1H3,(H,11,12)
  inchikey  = BSYNRYMUTXBXSQ-UHFFFAOYSA-N
  esmiles   = CC(=O)Oc1ccccc1C(=O)O theory{dft} xc{b3lyp} basis{6-311++G(2d,2p)} solvation_ty
  calculation_type = ovcn
  theory           = dft
  xc               = b3lyp
  basis            = 6-311++G(2d,2p)
  charge,mult      = 0 1
  energy           =    -648.912781 Hartrees
  enthalpy correct.=       0.169439 Hartrees
  entropy          =       109.438 cal/mol-K
  solvation energy =       -14.463 kcal/mol  solvation_type = COSMO
  Sitkoff cavity dispersion          =         2.657 kcal/mol
  Honig cavity dispersion            =         8.986 kcal/mol
  ASA solvent accesible surface area =       359.433 Angstrom2
  ASA solvent accesible volume       =       337.193 Angstrom3


  +-----------------+
  | Structural Data |
  +-----------------+
```



spin ON | spin OFF | labels On | labels Off | HOMO | LUMO | mo previous | mo next

JSmol: an open-source HTML5 viewer for chemical structures in 3D

JSmol: an open-source HTML5 viewer for chemical structures in 3D