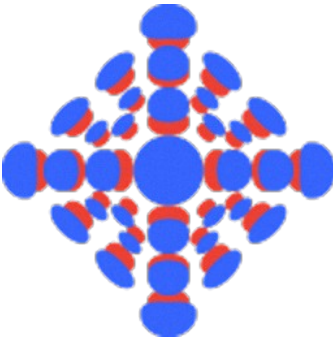




COSMOlogic TURBOMOLE 7.4 x64

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TmoleX 4.5.3N - defCOSMOthermJobTemplates

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Jobs running local: 0/3 remote: 0 Memory used for TmoleX: 57.0/69.2 MB System: 0.0/9588.9 MB

Geometry → Start Job → Results

Job Comparison Save as .jds Open as .jds

Project-Name
Batchjob-Name
Parentjob-Name
Job-Name
Formula
SMILES

2D structure

Number of atoms
Basis set
Symmetry
Charge
Multiplicity
Frozen core
Level of theory
RI
PNO
Dispersion
COSMO
COSMO-FBNC
Energy [kJ/mol]
HOMO-LUMO gap
Dipole moment
Dipole moment [D]

TmoleX

Version 4.5.3N (09/04/2020)

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defCOSMOthermJobTemplates

COSMO-AM1-SVP_3
COSMO_SVP_AM1
CH100

15
def-SVP
c1
-2.0
Singlet
off
DFT b-p
on
off

on
off

0.284218
from dscf

TmoleX 4.2 - DownloadLy.R

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ProjectList
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TmoleXProject
DownloadLy.R

Manage Job(s)

TmoleX

Version 4.2 (09/08/2016)

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