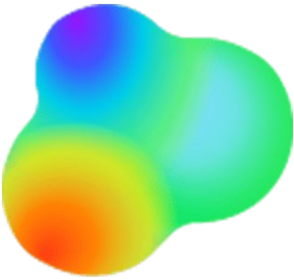




COSMOlogic COSMOthermX & TmoleX 19.0 x64

2025-07-10 16:53:25 label 我要反馈 下载页面



COSMOthermX - DownLoadLy.R.inpx

File Edit Compounds Run Result Extras Tools View License Help

Parameterization: BP_TZVP_19.cdd

Jobs

Project-List

Temp_Project

Your license information

COSMOthermX

Version 19.0.4

Revision 4825:4826

Installer date 14/08/2019

License expiration date 01-jul-2050

Customer : downloadly.ir

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product	licensed version
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cosmobase11	17
cosmoperm	19

Temp_Project: DownLoadLy.R

Compounds Properties .tab file

About COSMOthermX

COSMOthermX

Version 19.0.4 (14/08/2019) (Revision 4825:4826)

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TmoleX 4.5.3N - defCOSMOthermJobTemplates

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Open 3D Molecular Builder

Jobs running: local: 0/3 remote: 0

Memory used for TmoleX: 57.0/69.2 MB

System: 0.0/8588.9 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

R1

PNO

Dispersion

COSMO

COSMO-FDM

Energy [kJ/mol]

HOMO-LUMO gap [eV]

Dipole moment

Dipole moment [D]

from dcd

from dcd

TmoleX

Version 4.5.3N (09/04/2020)

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defCOSMOthermJobTemplates

COSMO-AM1-SVP_3

COSMO-SVP_AM1

C4H10O

15

def-SVP

c1

-2.0

Singlet

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DFT b-p

on

off

on

off

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