| surface | fcc | ua_sca | charmm_sca | availability | SMILES |
|---------|-----|--------|------------|--------------|--------|
| PEG | 000 | ALA | ALA | True | C |
| PEG | 000 | ARG | ARG | True | CCCNC(N)=[NH2+] |
| PEG | 000 | ASN | ASN | True | CC(N)=O |
| PEG | 000 | ASP | ASP | True | CC(=O)[O-] |
| PEG | 000 | AAN | ASPP | True | CC(=O)O |
| PEG | 000 | CYM | CYM | True | C[S-] |
| PEG | 000 | CYS | CYS | True | CS |
| PEG | 000 | GLN | GLN | True | CCC(N)=O |
| PEG | 000 | GLU | GLU | True | CCC(=O)[O-] |
| PEG | 000 | GAN | GLUP | True | CCC(=O)O |
| PEG | 000 | GLY | GLY | True | C |
| PEG | 000 | HIS | HIS | True | CC1CNCN1 |
| PEG | 000 | HID | HSD | True | CC1CNCN1 |
| PEG | 000 | HIE | HSE | True | CC1CNCN1 |
| PEG | 000 | HIP | HSP | True | CC1CNCN1 |
| PEG | 000 | ILE | ILE | True | CCCC |
| PEG | 000 | LEU | LEU | True | CC(C)C |
| PEG | 000 | LYS | LYS | True | CCCC[NH3+] |
| PEG | 000 | MET | MET | True | CCSC |
| PEG | 000 | PHE | PHE | True | CC1CCCCC1 |
| PEG | 000 | PRO | PRO | True | CCC |
| PEG | 000 | SER | SER | True | CO |
| PEG | 000 | THR | THR | True | CCO |
| PEG | 000 | TRP | TRP | True | CC1C[NH]C2CCCCC12 |
| PEG | 000 | TYR | TYR | True | CC1CCC(O)CC1 |
| PEG | 000 | VAL | VAL | True | CCC |