molfile

A molfile is a table containing atom type, connectivity and a more or less arbitrary *2D* or *3D* information about a molecule. Well-known file formats include the MOLfile used by MDL Information Systems Inc. (*e.g.*, in the database MACCS), the MOL2 file used by Tripos Associates (*e.g.*, in the modeling package SYBYL), or the CSSR format.

Source:
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1147

See also:
MOL file format
PAC, 1997, *69*, 1137 *(Glossary of terms used in computational drug design (IUPAC Recommendations 1997))* on page 1146