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Documents

915424 ► **Sigma-Aldrich.**

Benzene-d₆

≥95 atom % D, ≥99% (CP)

Synonym(s):

Hexadeuterobenzene

Empirical Formula (Hill Notation):

C₆D₆

CAS Number:

1076-43-3

Molecular Weight:

84.15

Beilstein/REAXYS Number:

1905426

MDL number:

MFCD00003010

PROPERTIES

isotopic purity	≥95 atom % D
assay	≥99% (CP)
refractive index	<i>n</i> ₂₀ /D 1.497 (lit.)
bp	79.1 °C/760 mmHg (lit.)
mp	6.8 °C (lit.)
density	0.950 g/mL at 25 °C (lit.)
mass shift	M+6
SMILES string	[2H]c1c([2H])c([2H])c([2H])c1[2H]
InChI	1S/C6H6/c1-2-4-6-5-3-1/h1-6H/i1D,2D,3D,4D,5D,6D
InChI key	UHOVQNZJYSORNB-MZWXYZOWSA-N

DESCRIPTION

Packaging

This product may be available from bulk stock and can be packaged on demand. For information on pricing, availability and packaging, please contact [Stable Isotopes Customer Service](#).

SAFETY INFORMATION

pictograms



GHS02,GHS07,GHS08

signalword

Danger

hcodes

H225 - H304 - H315 - H319 - H340 - H350 -
H372 - H412

pcodes

P201 - P210 - P273 - P301 + P310 + P331 -
P302 + P352 - P308 + P313

Target Organs

Blood

WGK Germany

WGK 3

Flash Point F

12.2 °F - closed cup

Flash Point C

-11 °C - closed cup