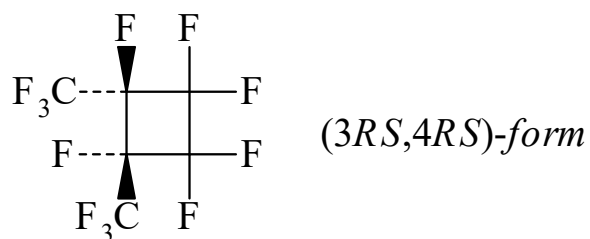




>>Entry Name: 1,1,2,2,3,4-Hexafluoro-3,4-bis(trifluoromethyl)cyclobutane, 9CI

Synonym(s): Perfluoro(1,2-dimethylcyclobutane)



CAS Registry Number: 2994-71-0

Related CAS Registry Numbers(s): 28677-00-1

Molecular Formula: C₆F₁₂

Molecular Weight: 300.047

Accurate Mass: 299.980836

Percentage Composition: C 24.02%; F 75.98%

Use/Importance: Taggant for detection of explosives. Refrigerant

>>Variant: (3RS,4RS)-form

Synonym(s): (±)-trans-form

CAS Registry Number: 3109-91-9

Molecular Formula: C₆F₁₂

Molecular Weight: 300.047

Percentage Composition: C 24.02%; F 75.98%

Melting Point: Fp -16.3°

Boiling Point: Bp 45.1°

Density: d₄²⁵ 1.673

Refractive Index: n_D²⁵ 1.2622

Other Data: Non-mutagenic

>>Variant: (3RS,4SR)-form

Synonym(s): cis-form

CAS Registry Number: 1858-56-6

Molecular Formula: C₆F₁₂

Molecular Weight: 300.047

Percentage Composition: C 24.02%; F 75.98%

Melting Point: Fp -50°

Boiling Point: Bp 43.6°

Density: d₄²⁵ 1.663

Refractive Index: n_D²⁵ 1.2600

Other Data: Non-mutagenic

References:

Brown, H.C., *J.O.C.*, 1957, **22**, 1256, (*synth, ir*)

Hauptschein, M. *et al.*, *J.A.C.S.*, 1958, **80**, 842, (*synth, F-19 nmr, ir*)

U.S. Pat., 1960, 2 957 032; *CA*, **55**, 18629a, (*synth*)

Atkinson, B. *et al.*, *J.C.S.(B)*, 1966, 740, (*ms, F-19 nmr*)

Davies, T. *et al.*, *J.C.S. Perkin I*, 1983, 109, (*synth*)