

Table of most likely compound densities.

This table represents the most likely range of values for a particular chemical compound. To use this table, first determine the heaviest element present in your compound. Find the nearest match in the table and read the lower and upper limits (quartiles). The density of your compound will most likely fall somewhere between these limits.

Data : The data is represented as the lower and upper Quartiles of the distribution of the densities of compounds, where that element is both present and is the heaviest element allowed for that set. The data is generated from the examination of 115,236 structures (each with $R \leq 0.05$, no errors and no disorder)(Cambridge Crystallographic Data Base, October 2002; Allen, F.H. 2002). Structures with no reported densities (density=0) were not included in the final distributions.

Element Type	Lower Quartile	Upper Quartile	Range g/cm ³	% of total
+ C	1.065 g/cm ³	1.295 g/cm ³	1.1 – 1.3	0.7
+ N	1.097	1.364	1.1 – 1.4	1.4
+ O	1.176	1.479	1.1 – 1.5	8.2
+ S	1.226	1.553	1.2 – 1.6	7.2
1 st row TR	1.275	1.873	1.3 – 1.9	3.9
+ Br	1.361	1.956	1.4 – 2.0	2.7
2 nd row TR	1.420	2.076	1.4 – 2.1	0.5
+ I	1.490	2.348	1.5 – 2.3	2.4
3 rd row TR	1.607	2.367	1.6 – 2.4	1.2
+ Pb	1.576	2.962	1.6 – 3.0	0.4

Allen F.H. "The Cambridge Structural Database: a quarter of a million crystal structures and rising." *Acta Cryst.* **B58**, 380-388, 2002

Compiled by J. H. Reibenspies, Department of Chemistry, Texas A & M University, copyright 2002