

To define the atom-atom potential of the intermolecular dispersion interaction the Buckingham–Corner potential is used

$$\varphi_{A...C_{\text{GTCB}}} = -\frac{C_1}{r^6} - \frac{C_2}{r^8} + B \cdot \exp(-3.57 \cdot r).$$

The atom-atom potential parameters for the interaction of various atoms *A* with the carbon atom of the GTCB C_{GTCB} .

	H [1]	C(<i>sp</i> ³) [1]	C(<i>sp</i> ²) [1]	N [2]	O [3]
$C_1 \cdot 10^{-3}$, kJ·Å ⁶ /mol	0.498	1.384	1.481	1.434	0.984
$C_2 \cdot 10^{-3}$, kJ·Å ⁸ /mol	0.947	2.149	2.300	3.913	1.627
$B \cdot 10^{-5}$, kJ/mol	0.360	1.889	2.021	1.378	0.723

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3. P. B. Dallakyan. Candidate Thesis in Chemical Sciences, Moscow State University, Moscow, 1982. [in Russian]