## Benson group additivity values ( $G A V \mathrm{~s}$ ) for common fragments found in organic molecules

| group | GAV <br> $\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ | group | GAV <br> $\left(\mathrm{kJ} \mathrm{mol}^{-1}\right)$ |
| :--- | :---: | :--- | :---: |
| $\mathrm{C}-(\mathrm{C})(\mathrm{H})_{3}$ | -41.8 | $\mathrm{C}-\left(\mathrm{C}_{\mathrm{d}}\right)(\mathrm{C})(\mathrm{H})_{2}$ | -20.1 |
| $\mathrm{C}-(\mathrm{C})_{2}(\mathrm{H})_{2}$ | -20.9 | $\mathrm{C}_{\mathrm{B}}-(\mathrm{H})$ | +13.8 |
| $\mathrm{C}-(\mathrm{C})_{3}(\mathrm{H})$ | -10.0 | $\mathrm{C}_{\mathrm{B}}-(\mathrm{C})$ | +23.0 |
| $\mathrm{C}-(\mathrm{C})_{4}$ | -0.4 | $\mathrm{C}_{\mathrm{d}}-(\mathrm{H})_{2}$ | +26.4 |
| $\mathrm{C}-\left(\mathrm{C}_{\mathrm{B}}\right)(\mathrm{H})_{3}$ | -41.8 | $\mathrm{C}_{\mathrm{d}}-(\mathrm{C})(\mathrm{H})$ | +36.0 |
| $\mathrm{C}-\left(\mathrm{C}_{\mathrm{B}}\right)(\mathrm{C})(\mathrm{H})_{2}$ | -19.2 | $\mathrm{C}_{\mathrm{d}}-(\mathrm{C})_{2}$ | +42.7 |
| $\mathrm{C}-\left(\mathrm{C}_{\mathrm{d}}\right)(\mathrm{H})_{3}$ | -41.8 |  |  |

(data from: N. Cohen, J. Phys. Chem. Ref. Data 1996, 25, 1411).
corrections

| gauche correction | $+3.3 \mathrm{~kJ} \mathrm{~mol}^{-1}$ |
| :--- | :--- |
| cis correction | $+4.6 \mathrm{~kJ} \mathrm{mo}^{-1}$ |
| ortho correction | $+2.5 \mathrm{~kJ} \mathrm{~mol}^{-1}$ |

## Atom types

"C" $\mathrm{sp}^{3}$-hybridized carbon as in common aliphatic hydrocarbons
" $\mathrm{C}_{\mathrm{B}}$ " $\mathrm{sp}^{2}$-hybridized carbon as in benzenoid hydrocarbons
" $\mathrm{C}_{\mathrm{d}}$ " $\mathrm{sp}^{2}$-hybridized carbon as in alkenes

