# DBGC数据库建立中用到的89种参考分子

DBGC数据库建立过程中用到的89种参考脂肪族分子被列举在下表1中。

表1 DBGC数据库建立过程中用到的89种参考脂肪族分子

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| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 1 | C3H7OH |  | -61.2±0.7 |
| 2 | C3H7OOH |  | -47.11 |
| 3 | C3H8 |  | -25.02±0.12 |
| 4 | C4H10 |  | -30.03±0.16 |
| 5 | C4H10 |  | -32.07±0.15 |
| 6 | C4H8 |  | -0.15±0.19 |
| 7 | C4H8 |  | -2.58±0.24 |
| 8 | C4H8 |  | -4.29±0.26 |
| 9 | C4H9OH |  | -66±1 |

续表1 DBGC数据库建立过程中用到的89种参考脂肪族分子

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| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 10 | C4H9OH |  | -67.8±0.2 |
| 11 | C4H9OH |  | -70.05 |
| 12 | C4H9OH |  | -74.72±0.21 |
| 13 | C4H9OOH |  | -56.14 |
| 14 | C5H10 |  | -1.97±0.28 |
| 15 | C5H10 |  | -5±2 |
| 16 | C5H10 |  | -7±1 |
| 17 | C5H10 |  | -7.7±0.4 |
| 18 | C5H10 |  | -6.09 |
| 19 | C5H10 |  | -8.39±0.2 |
| 20 | C5H10 |  | -9.92±0.21 |

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| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 21 | C5H10 |  | -18.26±0.19 |
| 22 | C5H12 |  | -35.08±0.14 |
| 23 | C5H12 |  | -36.73±0.14 |
| 24 | C5H12 |  | -40.14±0.15 |
| 25 | C6H12 |  | -11.82±0.16 |
| 26 | C6H12 |  | -14.79±0.21 |
| 27 | C6H12 |  | -15.18±0.21 |
| 28 | C6H12 |  | -15.74±0.36 |
| 29 | C6H12 |  | -16.8±0.36 |
| 30 | C6H12 |  | -13.4±0.21 |
| 31 | C6H12 |  | -29.78 |

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|  |  |  |  |
| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 32 | C6H12 |  | -10.2±0.6 |
| 33 | C6H12 |  | -25.33 |
| 34 | C6H12 |  | -6.6±0.2 |
| 35 | C6H12 |  | -11.2±0.26 |
| 36 | C6H12 |  | -12.2±0.2 |
| 37 | C6H12 |  | -11.8±0.24 |
| 38 | C6H12 |  | -11±0.2 |
| 39 | C6H14 |  | -39.94 |
| 40 | C6H14 |  | -41.66±0.25 |
| 41 | C6H14 |  | -41.02±0.23 |

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|  |  |  |  |
| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 42 | C6H14 |  | -42.49±0.24 |
| 43 | C6H14 |  | -44.35±0.23 |
| 44 | C7H14 |  | -15.1 |
| 45 | C7H14 |  | -16.9 |
| 46 | C7H14 |  | -36.99±0.25 |
| 47 | C7H14 |  | -30.37±0.25 |
| 48 | C7H14 |  | -17.7 |
| 49 | C7H14 |  | -33.05±0.28 |
| 50 | C7H14 |  | -30.96±0.32 |
| 51 | C7H14 |  | -31.93±0.35 |

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|  |  |  |  |
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| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 52 | C7H14 |  | -32.67±0.3 |
| 53 | C7H14 |  | -32.47±0.29 |
| 54 | C7H14 |  | -17.5 |
| 55 | C7H14 |  | -16.6 |
| 56 | C7H14 |  | -10.66±0.39 |
| 57 | C7H14 |  | -11.74±0.43 |
| 58 | C7H16 |  | -44.89±0.19 |
| 59 | C7H16 |  | -46.6±0.3 |
| 60 | C7H16 |  | -45.96±0.3 |
| 61 | C7H16 |  | -49.29±0.32 |

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|  |  |  |  |
| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 62 | C7H16 |  | -48.17±0.22 |
| 63 | C7H16 |  | -47.62±0.3 |
| 64 | C7H16 |  | -48.3±0.23 |
| 65 | C7H16 |  | -45.34±0.28 |
| 66 | C7H16 |  | -48.96±0.27 |
| 67 | C8H16 |  | -19.82 |
| 68 | C8H16 |  | -28.56 |
| 69 | C8H16 |  | -26.6 |
| 70 | C8H16 |  | -28.2 |

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| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 71 | C8H16 |  | -23.1 |
| 72 | C8H18 |  | -50.91±0.37 |
| 73 | C8H18 |  | -50.4±0.28 |
| 74 | C8H18 |  | -52.61±0.36 |
| 75 | C8H18 |  | -51.73±0.33 |
| 76 | C8H18 |  | -53.57±0.32 |
| 77 | C8H18 |  | -51.97±0.4 |
| 78 | C8H18 |  | -50.48±0.31 |

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|  |  |  |  |
| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 79 | C8H18 |  | -51.38±0.3 |
| 80 | C8H18 |  | -54.06 |
| 81 | C8H18 |  | -49.88 |
| 82 | C8H18 |  | -51.5±0.31 |
| 83 | C8H18 |  | -50.82±0.27 |
| 84 | C8H18 |  | -50.69±0.28 |
| 85 | C8H18 |  | -53.71±0.24 |
| 86 | C8H18 |  | -52.61±0.26 |
| 87 | C8H18 |  | -51.13±0.36 |
| 88 | C8H18 |  | -52.44±0.27 |

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|  |  |  |  |
| --- | --- | --- | --- |
| 编号 | 化学式 | 结构式 | 标准生成焓实验值（kcal/mol） |
| 89 | C8H18 |  | -53.21±0.36 |