### Trans

REMARK  Materials Studio PDB file  
REMARK  DMOL3 optimised structure, B3LYP/DNP 4.4 atomic basis set  
REMARK  Relative energy compared to a static trans conformation: ca -2.8 kJ mol⁻¹

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### Cis

REMARK  Materials Studio PCisDB file  
REMARK  DMOL3 optimised structure, B3LYP/DNP 4.4 atomic basis set  
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REMARK  Relative energy compared to a static trans conformation: ca -10.6 kJ mol⁻¹

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ATOM    14  C7  MOL     2      11.223   8.223   0.016  1.00  0.02           C
ATOM    15  H7A MOL     2      11.486   7.535  -0.775  1.00  0.02           H
ATOM    16  C8  MOL     2      10.110   9.015  -0.024  1.00  0.02           C
ATOM    17  C9  MOL     2       9.104   9.089  -1.074  1.00  0.02           C
ATOM    18  C10 MOL     2       9.303   8.235  -2.307  1.00  0.02           C
ATOM    19 AH10 MOL     2       9.192   7.178  -2.046  1.00  0.02           H
ATOM    20 BH10 MOL     2      10.324   8.362  -2.678  1.00  0.02           H
ATOM    21  C11 MOL     2       8.308   8.596  -3.419  1.00  0.02           C
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