

Pseudourea, 2-[2-(2-bornylamino)ethyl]-2-thio-, dihydrobromide

InChI: InChI=1S/C13H25N3S.2BrH/c1-12(2)9-4-5-13(12,3)10(8-9)16-6-7-17-11(14)15;;/h9-10,13-15,21-22,24-25,27-28,30-31,33-34,36-37,39-41,43-44,46-47,49-50,52-53,55-56,58-59,61-62,64-65,67-68,70-71,73-74,76-77,79-80,82-83,85-86,88-89,91-92,94-95,97-98,100-101,103-104,106-107,109-110,112-113,115-116,118-119,121-122,124-125,127-128,130-131,133-134,136-137,139-140,142-143,145-146,148-149,151-152,154-155,157-158,160-161,163-164,166-167,169-170,172-173,175-176,178-179,181-182,184-185,187-188,190-191,193-194,196-197,199-200,202-203,205-206,208-209,211-212,214-215,217-218,220-221,223-224,226-227,229-230,232-233,235-236,238-239,241-242,244-245,247-248,250-251,253-254,256-257,259-260,262-263,265-266,268-269,271-272,274-275,277-278,280-281,283-284,286-287,289-290,292-293,295-296,298-299,301-302,304-305,307-308,310-311,313-314,316-317,319-320,322-323,325-326,328-329,331-332,334-335,337-338,340-341,343-344,346-347,349-350,352-353,355-356,358-359,361-362,364-365,367-368,370-371,373-374,376-377,379-380,382-383,385-386,388-389,391-392,394-395,397-398,400-401,403-404,406-407,409-410,412-413,415-416,418-419,421-422,424-425,427-428,430-431,433-434,436-437,439-440,442-443,445-446,448-449,451-452,454-455,457-458,460-461,463-464,466-467,469-470,472-473,475-476,478-479,481-482,484-485,487-488,490-491,493-494,496-497,499-500,502-503,505-506,508-509,511-512,514-515,517-518,520-521,523-524,526-527,529-530,532-533,535-536,538-539,541-542,544-545,547-548,550-551,553-554,556-557,559-560,562-563,565-566,568-569,571-572,574-575,577-578,580-581,583-584,586-587,589-590,592-593,595-596,598-599,601-602,604-605,607-608,610-611,613-614,616-617,619-620,622-623,625-626,628-629,631-632,634-635,637-638,640-641,643-644,646-647,649-650,652-653,655-656,658-659,661-662,664-665,667-668,670-671,673-674,676-677,679-680,682-683,685-686,688-689,691-692,694-695,697-698,699,701,703,705,707,709,711,713,715,717,719,721,723,725,727,729,731,733,735,737,739,741,743,745,747,749,751,753,755,757,759,761,763,765,767,769,771,773,775,777,779,781,783,785,787,789,791,793,795,797,799,801,803,805,807,809,811,813,815,817,819,821,823,825,827,829,831,833,835,837,839,841,843,845,847,849,851,853,855,857,859,861,863,865,867,869,871,873,875,877,879,881,883,885,887,889,891,893,895,897,899,901,903,905,907,909,911,913,915,917,919,921,923,925,927,929,931,933,935,937,939,941,943,945,947,949,951,953,955,957,959,961,963,965,967,969,971,973,975,977,979,981,983,985,987,989,991,993,995,997,999

InchiKey: DRAAMCIERKTHFJ-UHFFFAOYSA-N
Formula: C13H27Br2N3S
SMILES: Br.Br.CC1(C)C2CCC1(C)C(NCCSC(=N)N)C2
Mol. weight [g/mol]: 417.25

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008413&Units=SI>

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