

Purine, 2-butylamino-6-methylamino

Inchi:	InChI=1S/C10H16N6/c1-3-4-5-12-10-15-8(11-2)7-9(16-10)14-6-13-7/h6H,3-5H2,1-2H3,(H
InchiKey:	VAQVKYREZCGXBS-UHFFFAOYSA-N
Formula:	C10H16N6
SMILES:	CCCCNc1nc(NC)c2[nH]cnc2n1
Mol. weight [g/mol]:	220.27
CAS:	5434-24-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.07		Crippen Method
logp	1.125		Crippen Method
mcvol	172.720	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5434242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/23-313-8/Purine-2-butylamino-6-methylamino.pdf>

Generated by Cheméo on 2025-12-05 14:49:17.613375513 +0000 UTC m=+4694355.143416168.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.