Benzyladenine

Other names:	124786-41-0 1H-Purin-6-amine, N-(phenylmethyl)- 3458-19-3 6-(Benzylamino)purine 6-(N-Benzylamino)purine 6-BA 6-BAP 6-Benzyladenine 9H-Purin-6-amine, N-(phenylmethyl)- 9H-Purine, 6-[(phenylmethyl)amino]- ABG 3034 Adenine, N-benzyl- BA BA (Growth stimulator) BA (growth stimulant) BAP BAP (growth stimulant) Benzylaminopurine Cytokinin B N-(Phenylmethyl)-1H-purin-6-amine N-(phenylmethyl)-9H-purin-6-amine N-Benzyl-9H-purin-6-amine N-Benzyladenine N6-Benzyladenine N6-Benzylaminopurine NSC 40818 Pro-Shear SD 4901 SQ 4609 Verdan senescence inhibitor benzyl(purin-6-yl)amine
Inchi:	InChI=1S/C12H11N5/c1-2-4-9(5-3-1)6-13-11-10-12(15-7-14-10)17-8-16-11/h1-5,7-8H,6H
InchiKey:	NWBJYWHLCVSVIJ-UHFFFAOYSA-N
Formula:	C12H11N5
SMILES:	c1ccc(CNc2ncnc3[nH]cnc23)cc1
Mol. weight [g/mol]:	225.25
CAS:	1214-39-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Aqueous Solubility Prediction Method
logp	1.483		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
rinpol	2527.00		NIST Webbook
tf	505.32	K	Aqueous Solubility Prediction Method
tf	503.15	K	Thermodynamic models for determination of solid liquid equilibrium of the 6-benzyladenine in pure and binary organic solvents

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1214397&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Thermodynamic models for determination of solid liquid equilibrium of the 6-benzyladenine in pure and binary organic solvents: https://www.doi.org/10.1016/j.jct.2016.12.002

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point