2-Pyrimidinecarbamonitrile, 4-methyl-

Inchi: InChI=1S/C6H6N4/c1-5-2-3-8-6(10-5)9-4-7/h2-3H,1H3,(H,8,9,10)
InchiKey: GRLTZYDMIBVIFT-UHFFFAOYSA-N
Formula: C6H6N4
SMILES: Cc1ccnc(NC#N)n1
Mol. weight [g/mol]: 134.14
CAS: 28732-65-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.85		Crippen Method
logp	0.678		Crippen Method
mcvol	102.960	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28732652&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

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