

Bupirimate

Other names: Sulfamic acid, N,N-dimethyl-, ester with 5-butyl-2-ethylamino-6-methylpyrimidin-4-ol
Inchi: InChI=1S/C13H24N4O3S/c1-6-8-9-11-10(3)15-13(14-7-2)16-12(11)20-21(18,19)17(4)5/h
InchiKey: DSKJPMWIHSOYEA-UHFFFAOYSA-N
Formula: C13H24N4O3S
SMILES: CCCCc1c(C)nc(NCC)nc1OS(=O)(=O)N(C)C
Mol. weight [g/mol]: 316.42
CAS: 58694-46-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	1.745		Crippen Method
mcvol	244.150	ml/mol	McGowan Method
rinpol	2202.00		NIST Webbook
rinpol	2202.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C58694465&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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