

Methotrexate

Other names:	L-Glutamic acid, N-[4-[(2,4-diamino-6-pteridiny)lmethyl]methylamino]benzoyl]-L-(+)-Amethopterin Glutamic acid, N-[p-[(2,4-diamino-6-pteridiny)lmethyl]methylamino]benzoyl]-, L-(+)- Amethopterin CL-14377 MTX NSC 740 R 9985 4-Amino-N10-methylpteroylglutamic acid 4-Amino-10-methylfolic acid (+)-Amethopterin L-Amethopterin Amethopterine Antifolan EMT 25,299 Glutamic acid, N-(p-(((2,4-diamino-6-pteridiny)lmethyl)methylamino)benzoyl)-, L-Hdmtx L-(+)-N-(p-(((2,4-Diamino-6-pteridiny)lmethyl)methylamino)benzoyl)glutamic acid Metatrexan Methotextrate Methylaminopterin N-(p-(((2,4-Diamino-6-pteridiny)lmethyl)methylamino)benzoyl)-L-(+)-glutamic acid N-(p-((2,4-Diamino-6-pteridyl)methyl)methylamino)benzoyl)glutamic acid, (L)- N-Bismethylpteroylglutamic acid NCI-C04671 X 133 Emtexate Kyselina 4-amino-N10-methylpteroylglutamova Kyselina N-(p-((2,4-diamino-6-pteridiny)lmethyl)methylamino)benzoyl)-L-glutamova Ledertrexate Methotrexat Methylaminopterinum Mexate Rheumatrex N-(4-[(2,4-Diamino-6-pteridiny)lmethyl](methyl)amino]benzoyl)glutamic acid, (L)- Methotrexat-Ebewe Trexall
Inchi:	InChI=1S/C20H22N8O5/c1-28(9-11-8-23-17-15(24-11)16(21)26-20(22)27-17)12-4-2-10(3)
InchiKey:	FBOZXECLQNJBKD-UHFFFAOYSA-N
Formula:	C20H22N8O5
SMILES:	CN(Cc1cnc2nc(N)nc(N)c2n1)c1ccc(C(=O)NC(CCC(=O)O)C(=O)O)cc1

Mol. weight [g/mol]: 454.44
CAS: 59-05-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	0.268		Crippen Method
mcvol	321.970	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C59052&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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