

4,5-Imidazoledicarboxylic acid

Other names:	Imidazole-4,5-dicarboxylic acid 1H-Imidazole-4,5-dicarboxylic acid «alpha», «beta»-Imidazoledicarboxylic acid Glyoxalinedicarboxylic acid 4,5-Dicarboxyimidazole 4,5-Imidazoledicarboxylate Glycoxalinedicarboxylic acid NSC 9236
Inchi:	InChI=1S/C5H4N2O4/c8-4(9)2-3(5(10)11)7-1-6-2/h1H,(H,6,7)(H,8,9)(H,10,11)
InchiKey:	ZEVWQFWTGHFIDH-UHFFFAOYSA-N
Formula:	C5H4N2O4
SMILES:	O=C(O)c1nc[nH]c1C(=O)O
Mol. weight [g/mol]:	156.10
CAS:	570-22-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.58		Crippen Method
logp	-0.676		Crippen Method
mvol	96.690	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C570229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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