Cytisine, N-formyl-

Other names: N-Formylcytisine
Inchi: InChI=1S/C12H14N2O2/c15-8-13-5-9-4-10(7-13)11-2-1-3-12(16)14(11)6-9/h1-3,8-10H,4-
InchiKey: PCYQRXYBKKZUSR-UHFFFAOYSA-N
Formula: C12H14N2O2
SMILES: O=CN1CC2CC(C1)c1cccc(=O)n1C2
Mol. weight [g/mol]: 218.25
CAS: 53007-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	0.424		Crippen Method
mcvol	161.860	ml/mol	McGowan Method
rinpol	2330.00		NIST Webbook
rinpol	2354.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2334.00		NIST Webbook
rinpol	2315.00		NIST Webbook

Sources

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=C53007060&Units=SI

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

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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