

Guaiapate

Inchi:	InChI=1S/C18H29NO4/c1-20-17-7-3-4-8-18(17)23-16-15-22-14-13-21-12-11-19-9-5-2-6-
InchiKey:	PPVFOZYARYOARE-UHFFFAOYSA-N
Formula:	C18H29NO4
SMILES:	COc1ccccc1OCCOCCOCCN1CCCCC1
Mol. weight [g/mol]:	323.43
CAS:	852-42-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.593		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		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=C852426&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

Latest version available from:

<https://www.chemeo.com/cid/62-462-0/Guaiapate.pdf>

Generated by Cheméo on 2025-12-06 01:00:21.150818398 +0000 UTC m=+4731018.680859062.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.