

CIRSILINEOL (5,4'-DIHYDROXY-6,7,3'-TRIMETHOXYFLAVONE)

Other names:	Cirsilineol
Inchi:	InChI=1S/C18H16O7/c1-22-13-6-9(4-5-10(13)19)12-7-11(20)16-14(25-12)8-15(23-2)18(2)
InchiKey:	VKOSQMWSWLZQPA-UHFFFAOYSA-N
Formula:	C18H16O7
SMILES:	COc1cc(-c2cc(=O)c3c(O)c(OC)c(OC)cc3o2)ccc1O
Mol. weight [g/mol]:	344.32

Physical Properties

Property code	Value	Unit	Source
logp	2.897		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
rinpol	3343.50		NIST Webbook
rinpol	3343.50		NIST Webbook
tf	490.11	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41365326&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.cheméo.com/cid/88-879-0/CIRSILINEOL-5-4-DIHYDROXY-6-7-3-TRIMETHOXYFLAVONE.pdf>

Generated by Cheméo on 2026-07-21 18:37:18.369318572 +0000 UTC m=+170134.211204037.

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