Myricetin

Inchi: InChI=1S/C15H10O8/c16-6-3-7(17)11-10(4-6)23-15(14(22)13(11)21)5-1-8(18)12(20)9(19
InchiKey: IKMDFBPHZNJCSN-UHFFFAOYSA-N
Formula: C15H10O8
SMILES: O=c1c(O)c(-c2cc(O)c(O)c(O)c2)oc2cc(O)cc(O)c12
Mol. weight [g/mol]: 318.24
CAS: 529-44-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Cheméo Relay (1.0)
logp	1.694		Crippen Method
mcvol	202.190	ml/mol	McGowan Method
tf	630.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

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):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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