CANNABICHROMENE

Other names:	2H-1-Benzopyran-5-ol, 2-methyl-2-(4-methyl-3-pentenyl)-7-pentyl-
	Cannabichrome
	Cannanbichromene
	Pentylcannabichromene
	Cannabichchromene
	2-Methyl-2-(4-methyl-3-pentenyl)-7-pentyl-2H-chromen-5-ol
	2H-1-Benzopyran-5-ol, 2-methyl-2-(4-methyl-3-pentenyl)-7-pentyl-, (.+/-.)-
	(.+/-.)-Cannabichromene
Inchi:	InChI=1S/C21H30O2/c1-5-6-7-10-17-14-19(22)18-11-13-21(4,23-20(18)15-17)12-8-9-16
InchiKey:	UVOLYTDXHDXWJU-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	CCCCCc1cc(O)c2c(c1)OC(C)(CCC=C(C)C)C=C2
Mol. weight [g/mol]:	314.47

Physical Properties

Property code	Value	Unit	Source
hfus	47.02	kJ/mol	Joback Method
logp	6.036		Crippen Method
mcvol	275.270	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.63	J/mol×K	838.54	Joback Method
cpg	880.20	J/mol×K	875.43	Joback Method
cpg	899.65	J/mol×K	912.32	Joback Method
cpg	919.22	J/mol×K	949.20	Joback Method
cpg	939.13	J/mol×K	986.09	Joback Method
cpg	959.60	J/mol×K	1022.98	Joback Method
cpg	980.87	J/mol×K	1059.87	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20675518&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume