

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:

CCCCC1cc(O)c2c(c1)OC(C)(CCC=C(C)C)C=C2

Mol. weight [g/mol]:

314.46

CAS:

20675-51-8

Physical Properties

Property code	Value	Unit	Source
gf	123.14	kJ/mol	Joback Method
hf	-325.40	kJ/mol	Joback Method
hfus	47.02	kJ/mol	Joback Method
hvap	82.73	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.036		Crippen Method
mcvol	275.270	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
tb	838.54	K	Joback Method
tc	1059.87	K	Joback Method
tf	536.22	K	Joback Method
vc	1.004	m ³ /kmol	Joback 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20675518&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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