

«DELTA»8-Tetrahydrocannabinol

Other names:

6H-Dibenzo[b,d]pyran-1-ol, 6a,7,10,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, (6aR,trans)-
6H-Dibenzo[b,d]pyran-1-ol, 6a,7,10,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, trans-(-)-
«DELTA»6-THC
«DELTA»1(6)-trans-Tetrahydrocannabinol
«DELTA»1(6)-Tetrahydrocannabinol
«DELTA»6-Tetrahydrocannabinol
«DELTA»8-trans-Tetrahydrocannabinol
(-)-«DELTA»6-Tetrahydrocannabinol
(-)-«DELTA»8-trans-Tetrahydrocannabinol
(-)-«DELTA»8-Tetrahydrocannabinol
Cannabinol, «DELTA»1(6)-tetrahydro-
«DELTA»8-THC
Cannabinol, 1-trans-«DELTA»8-tetrahydro-
1-trans-«DELTA»8-Tetrahydrocannabinol
6H-Dibenzo(b,d)pyran-1-ol, 6a,7,10,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, (6aR,10aR)-
(-)-«DELTA»6-3,4-trans-Tetrahydrocannabinol
(-)-trans-«DELTA»8-Tetrahydrocannabinol
«DELTA»8-I-Tetrahydrocannabinol
trans-«DELTA»8-Tetrahydrocannabinol
I-«DELTA»8-Tetrahydrocannabinol
8-Tetrahydrocannabinol
NSC 134453
«delta»-(sup6)-THC
«delta»-(sup8)-THC
(-)-«delta»-(sup8)-trans-Tetrahydrocannabinol
Cannabinol, 1-trans-«delta»-(sup8)-tetrahydro-
1-trans-«delta»-(sup8)-Tetrahydrocannabinol
6H-Dibenzo(b,d)pyran-1-ol, 6a,7,10,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-
6,6,9-Trimethyl-3-pentyl-6a,7,10,10a-tetrahydro-6H-benzo[c]chromen-1-ol

Inchi:

InChI=1S/C21H30O2/c1-5-6-7-8-15-12-18(22)20-16-11-14(2)9-10-17(16)21(3,4)23-19(20)

InchiKey:

HCAWPGARWVBULJ-UHFFFAOYSA-N

Formula:

C21H30O2

SMILES:

CCCCCc1cc(O)c2c(c1)OC(C)(C)C1CC=C(C)CC21

Mol. weight [g/mol]:

314.46

CAS:

5957-75-5

Physical Properties

Property code	Value	Unit	Source
gf	82.78	kJ/mol	Joback Method
hf	-398.00	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.736		Crippen Method
mcpvol	268.710	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2520.70		NIST Webbook
tb	845.82	K	Joback Method
tc	1074.44	K	Joback Method
tf	577.96	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.15	J/mol×K	845.82	Joback Method
cpg	899.14	J/mol×K	883.92	Joback Method
cpg	919.92	J/mol×K	922.03	Joback Method
cpg	940.71	J/mol×K	960.13	Joback Method
cpg	961.77	J/mol×K	998.23	Joback Method
cpg	983.32	J/mol×K	1036.33	Joback Method
cpg	1005.62	J/mol×K	1074.44	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C5957755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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