Dronabinol

Other names:

«DELTA»9-Tetrahydrocannabinol
6H-Dibenzo[b,d]pyran-1-ol, 6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, (6aR-trans)-
«DELTA»1-Tetrahydrocannabinol
«DELTA»1-THC
«DELTA»9-trans-Tetrahydrocannabinol
(-)-«DELTA»1-Tetrahydrocannabinol
(-)-«DELTA»9-trans-Tetrahydrocannabinol
(-)-«DELTA»9-Tetrahydrocannabinol
(-)-«DELTA»9-THC
(-)-trans-«DELTA»9-Tetrahydrocannabinol
(l)-«DELTA»1-Tetrahydrocannabinol
L-«DELTA»1-trans-Tetrahydrocannabinol
L-trans-«DELTA»9-Tetrahydrocannabinol
trans-«DELTA»9-Tetrahydrocannabinol, (-)-
Abbott 40566
Cannabinol, «DELTA»1-Tetrahydro-
SP 104
Tetrahydrocannabinol
«DELTA»9-THC
Cannabinol, 1-trans-«DELTA»9-tetrahydro-
QCD 84924
1-trans-«DELTA»9-tetrahydrocannabinol
6,6,9-Trimethyl-3-pentyl-7,8,9,10-tetrahydro-6H-dibenzo(b,d)pyran-1-ol
6H-Dibenzo(b,d)pyran-1-ol, 6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, (6aR,10aR)-
6H-Dibenzo(b,d)pyran-1-ol, 6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-, trans-
(6aR,10aR)-6a,7,8,10a-Tetrahydro-6,6,9-trimethyl-3-pentyl-6H-dibenzo[b,d]pyran-1-ol
Marinol
(-)-trans-«DELTA»1-Tetrahydrocannabinol
(-)-trans-«DELTA»9-THC
NSC-134454
Delta 9-THC
Delta-9-Tetrahydrocannabinol
6H-Dibenzo(b,d)pyran-1-ol, 6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-pentyl-
trans-«delta»9-Tetrahydrocannabinol
14C-«delta»1-Tetrahydrocannabinol
«delta»(sup9)-Thc
(-)-«delta»(sup9)-trans-Tetrahydrocannabinol
Cannabinol, 1-trans-«delta»(sup9)-tetrahydro-
1-trans-«delta»(sup9)-tetrahydrocannabinol
Primolut

	Exocyclic «delta»(9)(11)-Tetrahydrocannabiol
	6H-Dibenzo[b,d]pyran-1-ol, 6a,7,8,10a-tetrahydro-6,9,9-trimethyl-3-pentyl-, (6ar-trans)-
	6,6,9-Trimethyl-3-pentyl-6a,7,8,10a-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:	CYQFCXCEBYINGO-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	CCCCCc1cc(O)c2c(c1)OC(C)(C)C1CCC(C)=CC21
Mol. weight [g/mol]:	314.46
CAS:	1972-08-3

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
mcvol	268.710	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2473.00		NIST Webbook
tb	845.82	K	Joback Method
tc	1074.44	K	Joback Method
tf	577.96	K	Joback Method
vc	0.972	m3/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

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=C1972083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume