11-Hydroxy-«DELTA»9-tetrahydrocannabinol

Other names:	6H-Dibenzo[b,d]pyran-9-methanol, 6a,7,8,10a-tetrahydro-1-hydroxy-6,6-dimethyl-3-pentyl-, (6aR-trans)- 11-Hydroxy-«DELTA»9-THC 11-Hydroxytetrahydrocannabinol 7-Hydroxy-«DELTA»1-tetrahydrocannabinol 6H-Dibenzo(b,d)pyran-9-methanol, 6a,7,8,10a-tetrahydro-6,6-dimethyl-1-hydroxy-3-pentyl-,(6aR-trans)- 9-(Hydroxymethyl)-6,6-dimethyl-3-pentyl-6a,7,8,10a-tetrahydro-6H-benzo[c]chromen-1-ol, (6aR-trans)-
Inchi:	InChI=1S/C21H30O3/c1-4-5-6-7-14-11-18(23)20-16-10-15(13-22)8-9-17(16)21(2,3)24-19
InchiKey:	YCBKSSAWEUDACY-IRXDYDNUSA-N
Formula:	C21H30O3
SMILES:	CCCCCc1cc(O)c2c(c1)OC(C)(C)C1CCC(CO)=CC21
Mol. weight [g/mol]:	330.46
CAS:	36557-05-8

Physical Properties

Property code	Value	Unit	Source
gf	-54.04	kJ/mol	Joback Method
hf	-550.23	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	99.81	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.708		Crippen Method
mcvol	274.580	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	2902.70		NIST Webbook
rinpol	2902.70		NIST Webbook
tb	938.00	K	Joback Method
tc	1160.69	K	Joback Method
tf	638.78	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.12	J/mol×K	938.00	Joback Method

cpg	967.55	J/mol×K	975.12	Joback Method
cpg	988.32	J/mol×K	1012.23	Joback Method
cpg	1009.64	J/mol×K	1049.35	Joback Method
cpg	1031.75	J/mol×K	1086.46	Joback Method
cpg	1054.87	J/mol×K	1123.58	Joback Method
cpg	1079.22	J/mol×K	1160.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C36557058&Units=SI

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