Cannabinol

Other names: 3-Amyl-1-hydroxy-6,6,9-trimethyl-6H-dibenzo(b,d)pyran
6,6,9-Trimethyl-3-pentyl-6H-dibenzo(b,d)pyran-1-ol
6,6,9-trimethyl-3-pentyl-6H-benzo[c]chromen-1-ol
6H-Dibenzo[b,d]pyran-1-ol, 6,6,9-trimethyl-3-pentyl-
CBN

Inchi: InChI=1S/C21H26O2/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: VBGLYOIFKLUMQG-UHFFFAOYSA-N

Formula: C21H26O2

SMILES: CCCCCc1cc(O)c2c(c1)OC(C)(C)c1ccc(C)cc1-2

Mol. weight [g/mol]: 310.43

CAS: 521-35-7

Physical Properties

Property code	Value	Unit	Source
gf	138.86	kJ/mol	Joback Method
hf	-264.70	kJ/mol	Joback Method
hfus	44.37	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	5.728		Crippen Method
mcvol	260.110	ml/mol	McGowan Method
pc	1823.17	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2516.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2538.00		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2525.00		NIST Webbook
rinpol	2538.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	863.44	K	Joback Method
tc	1096.53	K	Joback Method
tf	613.00	K	Joback Method

vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.47	J/mol×K	863.44	Joback Method
cpg	831.52	J/mol×K	902.29	Joback Method
cpg	850.74	J/mol×K	941.14	Joback Method
cpg	870.39	J/mol×K	979.99	Joback Method
cpg	890.71	J/mol×K	1018.83	Joback Method
cpg	911.98	J/mol×K	1057.68	Joback Method
cpg	934.45	J/mol×K	1096.53	Joback Method
hfust	17.00	kJ/mol	352.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C521357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Cannabinol in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je100245n
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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