Hexahydrocannabinol

Other names: 6H-Dibenzo[b,d]pyran-1-ol, 6a,7,8,9,10,10a-hexahydro-6,6,9-trimethyl-3-pentyl-
Inchi: InChI=1S/C21H32O2/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: XKRHRBJLCLXSGE-UHFFFAOYSA-N
Formula: C21H32O2
SMILES: CCCCCc1cc(O)c2c(c1)OC(C)(C)C1CCC(C)CC21
Mol. weight [g/mol]: 316.48
CAS: 6692-85-9

Physical Properties

Property code	Value	Unit	Source
gf	54.74	kJ/mol	Joback Method
hf	-464.65	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	81.86	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.816		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2407.00		NIST Webbook
rinpol	2407.00		NIST Webbook
tb	837.01	K	Joback Method
tc	1063.38	K	Joback Method
tf	560.44	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.13	J/mol×K	837.01	Joback Method
cpg	932.17	J/mol×K	874.74	Joback Method
cpg	953.80	J/mol×K	912.47	Joback Method
cpg	975.28	J/mol×K	950.20	Joback Method
cpg	996.81	J/mol×K	987.93	Joback Method
cpg	1018.64	J/mol×K	1025.66	Joback Method

cpg	1041.00	J/mol×K	1063.38	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=C6692859&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume