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

Physical Properties

Property code	Value	Unit	Source
hfus	45.08	kJ/mol	Joback Method
logp	5.816		Crippen Method
mcvol	273.010	ml/mol	McGowan Method
rinpol	2407.00		NIST Webbook

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6692859&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices