6H-Dibenzo(b,d)pyran-1-ol, 3-hexyl-7,8,9,10-tetrahydro-6,6,9-trimethyl-

Other names: 3-Hexyl-7,8,9,10-tetrahydro-6,6,9-trimethyl-6H-dibenzo(b,d)pyran-1-ol
3-Homotetrahydrocannibinol
1-Hydroxy-3-n-hexyl-6,6,9-trimethyl-7,8,9,10-tetrahydro-6-dibenzopyran
Parahexyl
Pyrahexyl
Synhexyl

Inchi: InChI=1S/C22H32O2/c1-5-6-7-8-9-16-13-19(23)21-17-12-15(2)10-11-18(17)22(3,4)24-20

InchiKey: OORFXDSWECAQLI-UHFFFAOYSA-N

Formula: C22H32O2

SMILES: CCCCCCc1cc(O)c2c(c1)OC(C)(C)C1=C2CC(C)CC1

Mol. weight [g/mol]: 328.49

CAS: 117-51-1

Physical Properties

Property code	Value	Unit	Source
gf	89.28	kJ/mol	Joback Method
hf	-409.77	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	86.33	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.260		Crippen Method
mcvol	282.800	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	878.35	K	Joback Method
tc	1105.47	K	Joback Method
tf	605.99	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.31	J/mol×K	878.35	Joback Method

cpg	956.80	J/mol×K	916.20	Joback Method
cpg	978.27	J/mol×K	954.06	Joback Method
cpg	999.96	J/mol×K	991.91	Joback Method
cpg	1022.11	J/mol×K	1029.77	Joback Method
cpg	1044.97	J/mol×K	1067.62	Joback Method
cpg	1068.78	J/mol×K	1105.47	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=C117511&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