Nabilone

Other names:	9H-Dibenzo(b,d)pyran-9-one, 3-(1,1-dimethylheptyl)-6,6a,7,8,10,10a-hexahydro-1-hydroxy-6,6-dimethyl-, trans-(.+/-.)- LILLY 109514 (.+/-.)-3-(1,1-Dimethylheptyl-6,6a«beta»,7,8,10,10a«alpha»-hexahydro-1-hydroxy-6,6-dim Cesamet Compd. 109514 LY-109514 3-(1,1-Dimethylheptyl)-1-hydroxy-6,6-dimethyl-6,6a,7,8,10,10a-hexahydro-9H-benzo[c]ch
Inchi:	InChI=1S/C24H36O3/c1-6-7-8-9-12-23(2,3)16-13-20(26)22-18-15-17(25)10-11-19(18)24
InchiKey:	GECBBEABIDMGGL-UHFFFAOYSA-N
Formula:	C24H36O3
SMILES:	CCCCCCC(C)(C)c1cc(O)c2c(c1)OC(C)(C)C1CCC(=O)CC21
Mol. weight [g/mol]:	372.54
CAS:	51022-71-0

Physical Properties

Property code	Value	Unit	Source
gf	-32.04	kJ/mol	Joback Method
hf	-652.68	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.264		Crippen Method
mcvol	316.850	ml/mol	McGowan Method
pc	1366.68	kPa	Joback Method
rinpol	2945.60		NIST Webbook
rinpol	2945.60		NIST Webbook
tb	974.91	K	Joback Method
tc	1213.70	K	Joback Method
tf	669.13	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1136.90	J/mol×K	974.91	Joback Method
cpg	1161.61	J/mol×K	1014.71	Joback Method
cpg	1186.60	J/mol×K	1054.51	Joback Method
cpg	1212.13	J/mol×K	1094.30	Joback Method
cpg	1238.49	J/mol×K	1134.10	Joback Method
cpg	1265.96	J/mol×K	1173.90	Joback Method
cpg	1294.82	J/mol×K	1213.70	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C51022710&Units=SI
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

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

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