Tetrahydrocannabinol, TMS

Inchi: InChI=1S/C21H30O2/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: CYQFCXCEBYINGO-IRXDYDNUSA-N
Formula: C21H30O2
SMILES: CCCCCc1cc(O)c2c(c1)OC(C)(C)C1CCC(C)=CC21
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	82.78	kJ/mol	Joback Method
hf	-398.00	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	83.13	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.736		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	845.82	K	Joback Method
tc	1074.44	K	Joback Method
tf	577.96	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.15	J/mol×K	845.82	Joback Method
cpg	899.14	J/mol×K	883.92	Joback Method
cpg	919.92	J/mol×K	922.03	Joback Method
cpg	940.71	J/mol×K	960.13	Joback Method
cpg	961.77	J/mol×K	998.23	Joback Method
cpg	983.32	J/mol×K	1036.33	Joback Method
cpg	1005.62	J/mol×K	1074.44	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=R485893&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