Tetrahydrocannabinol

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: SJQJFSCMYCROHP-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: CCCCCC1CC2=C(c3cc(C)ccc3C(C)(C)O2)C(O)C1
Mol. weight [g/mol]: 314.46
CAS: 56282-24-7

Physical Properties

Property code	Value	Unit	Source
gf	90.95	kJ/mol	Joback Method
hf	-384.39	kJ/mol	Joback Method
hfus	42.76	kJ/mol	Joback Method
hvap	87.45	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.323		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2490.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2452.00		NIST Webbook
rinpol	2419.00		NIST Webbook
rinpol	2471.00		NIST Webbook
rinpol	2490.00		NIST Webbook
tb	862.36	K	Joback Method
tc	1075.33	K	Joback Method
tf	539.58	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.36	J/mol×K	862.36	Joback Method
cpg	902.49	J/mol×K	897.86	Joback Method
cpg	921.24	J/mol×K	933.35	Joback Method
cpg	939.77	J/mol×K	968.85	Joback Method
cpg	958.22	J/mol×K	1004.34	Joback Method
cpg	976.76	J/mol×K	1039.84	Joback Method
cpg	995.53	J/mol×K	1075.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56282247&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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