exo-THC

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: AOYYFUGUUIRBML-UHFFFAOYSA-N
Formula: C21H30O2
SMILES: C=C1CCC2C(C1)c1c(O)cc(CCCCC)cc1OC2(C)C
Mol. weight [g/mol]: 314.46
CAS: 27179-28-8

Physical Properties

Property code	Value	Unit	Source
gf	115.53	kJ/mol	Joback Method
hf	-360.07	kJ/mol	Joback Method
hfus	42.85	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.736		Crippen Method
mcvol	268.710	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2499.80		NIST Webbook
rinpol	2499.80		NIST Webbook
tb	840.84	K	Joback Method
tc	1068.58	K	Joback Method
tf	578.36	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.83	J/mol×K	840.84	Joback Method
cpg	898.83	J/mol×K	878.80	Joback Method
cpg	919.56	J/mol×K	916.75	Joback Method
cpg	940.24	J/mol×K	954.71	Joback Method
cpg	961.11	J/mol×K	992.67	Joback Method
cpg	982.41	J/mol×K	1030.62	Joback Method
cpg	1004.37	J/mol×K	1068.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27179288&Units=SI

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