(-)-Cannabidiol

Other names:	1,3-Benzenediol, 2-[3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-5-pentyl-, (1R-trans)- Cannabidiol
Inchi:	InChI=1S/C21H30O2/c1-5-6-7-8-16-12-19(22)21(20(23)13-16)18-11-15(4)9-10-17(18)14
InchiKey:	QHMBSVQNZZTUGM-ZWKOTPCHSA-N
Formula:	C21H30O2
SMILES:	C=C(C)C1CCC(C)=CC1c1c(O)cc(CCCCC)cc1O
Mol. weight [g/mol]:	314.46
CAS:	13956-29-1

Physical Properties

Property code	Value	Unit	Source
gf	35.84	kJ/mol	Joback Method
hf	-410.40	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.846		Crippen Method
mcvol	275.270	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
tb	888.36	K	Joback Method
tc	1119.73	K	Joback Method
tf	589.51	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.02	J/mol×K	888.36	Joback Method
cpg	920.75	J/mol×K	926.92	Joback Method
cpg	938.84	J/mol×K	965.48	Joback Method
cpg	956.45	J/mol×K	1004.05	Joback Method
cpg	973.76	J/mol×K	1042.61	Joback Method

cpg	990.91	J/mol×K	1081.17	Joback Method
cpg	1008.09	J/mol×K	1119.73	Joback Method
hfust	28.40	kJ/mol	340.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13956291&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
hfust:	Enthalpy of fusion at a given temperature
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