11-nor-D9-Tetrahydrocannabinol-9-carboxylic acid

Inchi: InChI=1S/C20H26O4/c1-3-4-5-6-13-9-17(21)19-16-11-14(20(22)23)7-8-15(16)12(2)24-18

InchiKey: JUOBYKAWBVCAIM-UHFFFAOYSA-N

Formula: C20H26O4

SMILES: CCCCCc1cc(O)c2c(c1)OC(C)C1CCC(C(=O)O)=CC21

Mol. weight [g/mol]: 330.42

Physical Properties

Property code	Value	Unit	Source
gf	-185.89	kJ/mol	Joback Method
hf	-657.41	kJ/mol	Joback Method
hfus	54.24	kJ/mol	Joback Method
hvap	105.48	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.410		Crippen Method
mcvol	262.060	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	2762.00		NIST Webbook
rinpol	2762.00		NIST Webbook
tb	968.75	K	Joback Method
tc	1195.41	K	Joback Method
tf	653.54	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.81	J/mol×K	968.75	Joback Method
cpg	914.13	J/mol×K	1006.53	Joback Method
cpg	928.98	J/mol×K	1044.30	Joback Method
cpg	943.49	J/mol×K	1082.08	Joback Method
cpg	957.79	J/mol×K	1119.86	Joback Method
cpg	972.01	J/mol×K	1157.63	Joback Method
cpg	986.30	J/mol×K	1195.41	Joback Method
dvisc	0.0000567	Pa×s	653.54	Joback Method

dvisc	0.0000292	Pa×s	706.07	Joback Method
dvisc	0.0000165	Pa×s	758.61	Joback Method
dvisc	0.0000100	Pa×s	811.14	Joback Method
dvisc	0.0000065	Pa×s	863.68	Joback Method
dvisc	0.0000044	Pa×s	916.21	Joback Method
dvisc	0.0000031	Pa×s	968.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R22360&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
dvisc:	Dynamic viscosity
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