Licarin A

Inchi: InChI=1S/C20H22O4/c1-5-6-13-9-15-12(2)19(24-20(15)18(10-13)23-4)14-7-8-16(21)17(1
InchiKey: ITDOFWOJEDZPCF-AATRIKPKSA-N
Formula: C20H22O4
SMILES: CC=Cc1cc(OC)c2c(c1)C(C)C(c1ccc(O)c(OC)c1)O2
Mol. weight [g/mol]: 326.39
CAS: 51020-86-1

Physical Properties

Property code	Value	Unit	Source
gf	-13.66	kJ/mol	Joback Method
hf	-433.02	kJ/mol	Joback Method
hfus	49.63	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.680		Crippen Method
mcvol	253.460	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	2722.90		NIST Webbook
rinpol	2722.90		NIST Webbook
tb	888.92	K	Joback Method
tc	1126.95	K	Joback Method
tf	609.45	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.21	J/mol×K	888.92	Joback Method
cpg	810.09	J/mol×K	928.59	Joback Method
cpg	825.15	J/mol×K	968.26	Joback Method
cpg	839.51	J/mol×K	1007.94	Joback Method
cpg	853.29	J/mol×K	1047.61	Joback Method
cpg	866.60	J/mol×K	1087.28	Joback Method
cpg	879.56	J/mol×K	1126.95	Joback Method

dvisc	0.0000779	Pa×s	609.45	Joback Method
dvisc	0.0000475	Pa×s	656.03	Joback Method
dvisc	0.0000309	Pa×s	702.61	Joback Method
dvisc	0.0000212	Pa×s	749.19	Joback Method
dvisc	0.0000152	Pa×s	795.76	Joback Method
dvisc	0.0000113	Pa×s	842.34	Joback Method
dvisc	0.0000087	Pa×s	888.92	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=C51020861&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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