2(3H)-Furanone, 3,4-bis(1,3-benzodioxol-5-ylmethyl)dihydro-, (3R-trans)-

Other names: 2(3H)-Furanone, dihydro-3,4-dipiperonyl-, trans-(-)-
Cubebinolide
Hinokinin
(3R,4R)-3,4-bis(Benzo[d][1,3]dioxol-5-ylmethyl)dihydrofuran-2(3H)-one

Inchi: InChI=1S/C20H18O6/c21-20-15(6-13-2-4-17-19(8-13)26-11-24-17)14(9-22-20)5-12-1-3-1

InchiKey: DDWGQGZPYDSYEL-LSDHHAIUSA-N

Formula: C20H18O6

SMILES: O=C1OCC(Cc2ccc3c(c2)OCO3)C1Cc1ccc2c(c1)OCO2

Mol. weight [g/mol]: 354.35

CAS: 26543-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-83.61	kJ/mol	Joback Method
hf	-600.23	kJ/mol	Joback Method
hfus	62.62	kJ/mol	Joback Method
hvap	94.50	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	2.718		Crippen Method
mcvol	243.480	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	3096.20		NIST Webbook
rinpol	3096.20		NIST Webbook
tb	966.28	K	Joback Method
tc	1230.68	K	Joback Method
tf	670.17	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.89	J/mol×K	966.28	Joback Method
cpg	837.98	J/mol×K	1010.35	Joback Method
cpg	850.93	J/mol×K	1054.41	Joback Method

cpg	862.87	J/mol×K	1098.48	Joback Method
cpg	873.97	J/mol×K	1142.55	Joback Method
cpg	884.36	J/mol×K	1186.62	Joback Method
cpg	894.20	J/mol×K	1230.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26543895&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

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