(3R,4R)-3,4-bis(3,4,5-Trimethoxybenzyl)dihydrofu

Inchi: InChI=1S/C24H30O8/c1-26-18-9-14(10-19(27-2)22(18)30-5)7-16-13-32-24(25)17(16)8-1
InchiKey: VUNCHONBJWJYID-SJORKVTESA-N
Formula: C24H30O8
SMILES: COc1cc(CC2COC(=O)C2Cc2cc(OC)c(OC)c(OC)c2)cc(OC)c1OC
Mol. weight [g/mol]: 446.49
CAS: 93395-16-5

Physical Properties

Property code	Value	Unit	Source
gf	-491.63	kJ/mol	Joback Method
hf	-1157.33	kJ/mol	Joback Method
hfus	53.29	kJ/mol	Joback Method
hvap	100.71	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.313		Crippen Method
mcvol	333.300	ml/mol	McGowan Method
pc	1206.47	kPa	Joback Method
rinpol	3348.20		NIST Webbook
rinpol	3348.20		NIST Webbook
tb	1071.66	K	Joback Method
tc	1314.52	K	Joback Method
tf	723.03	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.58	J/mol×K	1071.66	Joback Method
cpg	1150.10	J/mol×K	1112.14	Joback Method
cpg	1154.44	J/mol×K	1152.61	Joback Method
cpg	1155.50	J/mol×K	1193.09	Joback Method
cpg	1153.19	J/mol×K	1233.57	Joback Method
cpg	1147.38	J/mol×K	1274.05	Joback Method
cpg	1137.99	J/mol×K	1314.52	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=C93395165&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