(2R,3R,4R,5R)-3,4-Dimethyl-2,5-bis(3,4,5-trimethox

Inchi: InChI=1S/C24H32O7/c1-13-14(2)22(16-11-19(27-5)24(30-8)20(12-16)28-6)31-21(13)15-
InchiKey: ZPINJJOPURFFNV-WJWAULOUSA-N
Formula: C24H32O7
SMILES: COc1cc(C2OC(c3cc(OC)c(OC)c(OC)c3)C(C)C2C)cc(OC)c1OC
Mol. weight [g/mol]: 432.51
CAS: 50393-99-2

Physical Properties

Property code	Value	Unit	Source
gf	-384.46	kJ/mol	Joback Method
hf	-1060.31	kJ/mol	Joback Method
hfus	55.92	kJ/mol	Joback Method
hvap	95.84	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.823		Crippen Method
mcvol	331.730	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	3131.70		NIST Webbook
rinpol	3131.70		NIST Webbook
tb	994.50	K	Joback Method
tc	1223.51	K	Joback Method
tf	646.33	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.93	J/mol×K	994.50	Joback Method
cpg	1147.28	J/mol×K	1032.67	Joback Method
cpg	1158.12	J/mol×K	1070.84	Joback Method
cpg	1166.37	J/mol×K	1109.01	Joback Method
cpg	1171.96	J/mol×K	1147.17	Joback Method
cpg	1174.84	J/mol×K	1185.34	Joback Method
cpg	1174.92	J/mol×K	1223.51	Joback Method

dvisc	0.0001419	Pa×s	646.33	Joback Method
dvisc	0.0001038	Pa×s	704.36	Joback Method
dvisc	0.0000796	Pa×s	762.39	Joback Method
dvisc	0.0000634	Pa×s	820.41	Joback Method
dvisc	0.0000520	Pa×s	878.44	Joback Method
dvisc	0.0000437	Pa×s	936.47	Joback Method
dvisc	0.0000375	Pa×s	994.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50393992&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