1,7-bis(3,4-Dimethoxyphenyl)heptane-3,5-diyl diacetate

Inchi: InChI=1S/C27H36O8/c1-18(28)34-22(11-7-20-9-13-24(30-3)26(15-20)32-5)17-23(35-19(
InchiKey: HHLUMCLAOIMUOP-UHFFFAOYSA-N
Formula: C27H36O8
SMILES: COc1ccc(CCC(CC(CCc2ccc(OC)c(OC)c2)OC(C)=O)OC(C)=O)cc1OC
Mol. weight [g/mol]: 488.57

Physical Properties

Property code	Value	Unit	Source
gf	-529.96	kJ/mol	Joback Method
hf	-1202.47	kJ/mol	Joback Method
hfus	55.49	kJ/mol	Joback Method
hvap	110.07	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.540		Crippen Method
mcvol	382.130	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	3347.30		NIST Webbook
rinpol	3347.30		NIST Webbook
tb	1131.82	K	Joback Method
tc	1388.55	K	Joback Method
tf	700.21	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.59	J/mol×K	1131.82	Joback Method
cpg	1294.22	J/mol×K	1345.76	Joback Method
cpg	1300.26	J/mol×K	1302.97	Joback Method
cpg	1303.07	J/mol×K	1260.19	Joback Method
cpg	1302.71	J/mol×K	1217.40	Joback Method
cpg	1299.20	J/mol×K	1174.61	Joback Method
cpg	1284.92	J/mol×K	1388.55	Joback Method
dvisc	0.0000053	Pa×s	1131.82	Joback Method

dvisc	0.0000067	Pa×s	1059.88	Joback Method
dvisc	0.0000088	Pa×s	987.95	Joback Method
dvisc	0.0000121	Pa×s	916.01	Joback Method
dvisc	0.0000177	Pa×s	844.08	Joback Method
dvisc	0.0000275	Pa×s	772.14	Joback Method
dvisc	0.0000469	Pa×s	700.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412828&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