1,7-bis(4-Hydroxy-3-methoxyphenyl)heptane-3,5-diacetate

InChI: InChI=1S/C25H32O8/c1-16(26)32-20(9-5-18-7-11-22(28)24(13-18)30-3)15-21(33-17(2)2
InchiKey: DRDZHMFYPWLHJH-UHFFFAOYSA-N
Formula: C25H32O8
SMILES: COc1cc(CCC(CC(CCc2ccc(O)c(OC)c2)OC(C)=O)OC(C)=O)ccc1O
Mol. weight [g/mol]: 460.52
CAS: 135308-88-2

Physical Properties

Property code	Value	Unit	Source
gf	-626.78	kJ/mol	Joback Method
hf	-1228.43	kJ/mol	Joback Method
hfus	60.28	kJ/mol	Joback Method
hvap	125.50	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.934		Crippen Method
mcvol	353.950	ml/mol	McGowan Method
pc	1463.49	kPa	Joback Method
rinpol	3340.30		NIST Webbook
rinpol	3340.30		NIST Webbook
tb	1192.50	K	Joback Method
tc	1461.30	K	Joback Method
tf	831.61	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.78	J/mol×K	1192.50	Joback Method
cpg	1256.32	J/mol×K	1237.30	Joback Method
cpg	1271.33	J/mol×K	1282.10	Joback Method
cpg	1285.99	J/mol×K	1326.90	Joback Method
cpg	1300.46	J/mol×K	1371.70	Joback Method
cpg	1314.91	J/mol×K	1416.50	Joback Method
cpg	1329.52	J/mol×K	1461.30	Joback Method

dvisc	0.0000002	Pa×s	831.61	Joback Method
dvisc	7.4636808e-08	Pa×s	891.76	Joback Method
dvisc	4.0262509e-08	Pa×s	951.91	Joback Method
dvisc	2.3372776e-08	Pa×s	1012.05	Joback Method
dvisc	1.4421796e-08	Pa×s	1072.20	Joback Method
dvisc	9.3670998e-09	Pa×s	1132.35	Joback Method
dvisc	6.3547265e-09	Pa×s	1192.50	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=C135308882&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