(3R,5S)-1-(4-Hydroxy-3-methoxyphenyl)decane-3,diacetate

InChI: InChI=1S/C21H32O6/c1-5-6-7-8-18(26-15(2)22)14-19(27-16(3)23)11-9-17-10-12-20(24)2

InChIKey: PXBFKEHWQRAQQD-UHFFFAOYSA-N

Formula: C21H32O6

SMILES: CCCCCC(CC(CCc1ccc(O)c(OC)c1)OC(C)=O)OC(C)=O

Mol. weight [g/mol]: 380.48

CAS: 143615-75-2

Physical Properties

Property code	Value	Unit	Source
gf	-503.62	kJ/mol	Joback Method
hf	-1061.40	kJ/mol	Joback Method
hfus	49.30	kJ/mol	Joback Method
hvap	98.24	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.167		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2536.10		NIST Webbook
rinpol	2536.10		NIST Webbook
tb	966.28	K	Joback Method
tc	1185.69	K	Joback Method
tf	613.64	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.32	J/mol×K	966.28	Joback Method
cpg	1089.07	J/mol×K	1149.13	Joback Method
cpg	1078.08	J/mol×K	1112.56	Joback Method
cpg	1066.16	J/mol×K	1075.99	Joback Method
cpg	1053.26	J/mol×K	1039.42	Joback Method
cpg	1039.34	J/mol×K	1002.85	Joback Method
cpg	1099.20	J/mol×K	1185.69	Joback Method

dvisc	0.0000010	Pa×s	966.28	Joback Method
dvisc	0.0000015	Pa×s	907.51	Joback Method
dvisc	0.0000023	Pa×s	848.73	Joback Method
dvisc	0.0000039	Pa×s	789.96	Joback Method
dvisc	0.0000069	Pa×s	731.19	Joback Method
dvisc	0.0000137	Pa×s	672.41	Joback Method
dvisc	0.0000310	Pa×s	613.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C143615752&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
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