(2R,3R)-2,3-Bis[(3-(acetyl)oxyphenyl)methyl]butan diacetate

Other names: Enterodiol, tetra(acetate)
Inchi: InChI=1S/C26H30O8/c1-17(27)31-15-23(11-21-7-5-9-25(13-21)33-19(3)29)24(16-32-18(
InchiKey: JQSSCWWDRPKOGE-UHFFFAOYSA-N
Formula: C26H30O8
SMILES: CC(=O)OCC(Cc1cccc(OC(C)=O)c1)C(COC(C)=O)Cc1cccc(OC(C)=O)c1
Mol. weight [g/mol]: 470.51

Physical Properties

Property code	Value	Unit	Source
gf	-566.96	kJ/mol	Joback Method
hf	-1119.61	kJ/mol	Joback Method
hfus	54.50	kJ/mol	Joback Method
hvap	115.19	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	3.681		Crippen Method
mcvol	359.440	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	1161.88	K	Joback Method
tc	1423.50	K	Joback Method
tf	719.30	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1189.45	J/mol×K	1161.88	Joback Method
cpg	1190.13	J/mol×K	1379.89	Joback Method
cpg	1194.86	J/mol×K	1336.29	Joback Method
cpg	1197.18	J/mol×K	1292.69	Joback Method
cpg	1197.06	J/mol×K	1249.09	Joback Method
cpg	1194.49	J/mol×K	1205.48	Joback Method
cpg	1183.02	J/mol×K	1423.50	Joback Method

dvisc	0.0000093	Pa×s	1161.88	Joback Method
dvisc	0.0000120	Pa×s	1088.12	Joback Method
dvisc	0.0000159	Pa×s	1014.35	Joback Method
dvisc	0.0000222	Pa×s	940.59	Joback Method
dvisc	0.0000326	Pa×s	866.83	Joback Method
dvisc	0.0000516	Pa×s	793.06	Joback Method
dvisc	0.0000897	Pa×s	719.30	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=U378737&Units=SI

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