2-CO2Me-3,4-(OH)2-4'-OMe-bibenzyl, acetylated

Inchi: InChI=1S/C21H22O7/c1-13(22)27-18-12-9-16(8-5-15-6-10-17(25-3)11-7-15)19(21(24)26
InchiKey: JRJJBYUGAJBEKT-UHFFFAOYSA-N
Formula: C21H22O7
SMILES: COC(=O)c1c(CCc2ccc(OC)cc2)ccc(OC(C)=O)c1OC(C)=O
Mol. weight [g/mol]: 386.40

Physical Properties

Property code	Value	Unit	Source
gf	-494.52	kJ/mol	Joback Method
hf	-916.21	kJ/mol	Joback Method
hfus	46.22	kJ/mol	Joback Method
hvap	99.42	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.118		Crippen Method
mcvol	287.420	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	1004.45	K	Joback Method
tc	1237.61	K	Joback Method
tf	668.06	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.78	J/mol×K	1004.45	Joback Method
cpg	905.27	J/mol×K	1043.31	Joback Method
cpg	912.99	J/mol×K	1082.17	Joback Method
cpg	918.90	J/mol×K	1121.03	Joback Method
cpg	923.00	J/mol×K	1159.89	Joback Method
cpg	925.26	J/mol×K	1198.75	Joback Method
cpg	925.67	J/mol×K	1237.61	Joback Method
dvisc	0.0001509	Pa×s	668.06	Joback Method

dvisc	0.0001020	Pa×s	724.12	Joback Method
dvisc	0.0000730	Pa×s	780.19	Joback Method
dvisc	0.0000546	Pa×s	836.26	Joback Method
dvisc	0.0000424	Pa×s	892.32	Joback Method
dvisc	0.0000339	Pa×s	948.38	Joback Method
dvisc	0.0000278	Pa×s	1004.45	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=R273853&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