9-Hydroxymegastigma-4,6-dien-3-one (isomer # 2), «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C27H26F12O11/c1-10-7-12(40)8-23(3,4)13(10)6-5-11(2)46-18-17(50-22(44)27

InchiKey: GDLXSXLMGJXZHJ-YDIZBRRMSA-N

Formula: C27H26F12O11

SMILES: CC1=CC(=O)CC(C)(C)C1=CCC(C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC

Mol. weight [g/mol]: 754.47

Physical Properties

Property code	Value	Unit	Source
hfus	72.10	kJ/mol	Joback Method
logp	4.906		Crippen Method
mcvol	425.280	ml/mol	McGowan Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1602.14	J/mol×K	1248.83	Joback Method
cpg	1618.69	J/mol×K	1306.93	Joback Method
cpg	1634.10	J/mol×K	1365.04	Joback Method
cpg	1648.84	J/mol×K	1423.14	Joback Method
cpg	1663.41	J/mol×K	1481.25	Joback Method
cpg	1678.30	J/mol×K	1539.35	Joback Method
cpg	1694.01	J/mol×K	1597.45	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R184748&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices