9-Hydroxymegastigma-4,6-dien-3-one (isomer # 2), 6-O-(«alpha»-arabinofuranosyl)-«beta»-D-glucopy TFA

Inchi: InChI=1S/C36H32F18O17/c1-11-7-13(55)8-30(3,4)14(11)6-5-12(2)64-23-21(71-29(61)36

InchiKey: GWVVFIFXYLPPRJ-KARAQSPQSA-N

Formula: C36H32F18O17

SMILES: CC1=CC(=O)CC(C)(C)C1=CCC(C)OC1OC(COC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)

Mol. weight [g/mol]: 1078.60

Physical Properties

Property code	Value	Unit	Source
hfus	110.95	kJ/mol	Joback Method
logp	5.596		Crippen Method
mcvol	578.470	ml/mol	McGowan Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2205.47	J/mol×K	1647.13	Joback Method
cpg	2208.10	J/mol×K	1834.09	Joback Method
cpg	2227.92	J/mol×K	2021.05	Joback Method
cpg	2283.16	J/mol×K	2208.01	Joback Method
cpg	2392.07	J/mol×K	2394.97	Joback Method
cpg	2572.92	J/mol×K	2581.93	Joback Method
cpg	2843.93	J/mol×K	2768.89	Joback Method

Sources

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=R184733&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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