

Pentosyl «beta»-D-glucopyranoside of methyl salicylate, isomer # 2, TFA

Inchi: InChI=1S/C22H14F12O12/c1-40-13(35)7-4-2-3-5-8(7)42-14-12(46-18(39)22(32,33)34)11
InchiKey: NWJNOOFMDOXMLR-ZAOAHOKWSA-N
Formula: C22H14F12O12
SMILES: COC(=O)c1ccccc1OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1
Mol. weight [g/mol]: 698.32

Physical Properties

Property code	Value	Unit	Source
hfus	72.91	kJ/mol	Joback Method
log10ws	-6.20		Cheméo Relay (1.0)
logp	3.105		Crippen Method
mcvol	356.400	ml/mol	McGowan Method
rinpol	2545.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.27	J/mol×K	1144.43	Joback Method
cpg	1230.21		1192.42	Joback Method
cpg	1227.04		1240.41	Joback Method
cpg	1220.82		1288.39	Joback Method
cpg	1211.64		1336.38	Joback Method
cpg	1199.58		1384.37	Joback Method
cpg	1184.71		1432.36	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=R330491&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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