

furan linalyloxide «beta»-D-glucopyranoside (Z/ E), TFA

Inchi:	InChI=1S/C24H24F12O11/c1-5-20(4)7-6-10(46-20)19(2,3)47-14-13(45-18(40)24(34,35)3
InchiKey:	WJLOKMGYFMOJBB-ZIXXQERISA-N
Formula:	C24H24F12O11
SMILES:	C=CC1(C)CCC(C(C)(C)OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F
Mol. weight [g/mol]:	716.42

Physical Properties

Property code	Value	Unit	Source
hfus	69.65	kJ/mol	Joback Method
logp	4.158		Crippen Method
mcvol	391.610	ml/mol	McGowan Method
rinpol	1777.00		NIST Webbook
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1467.29	J/mol×K	1113.49	Joback Method
cpg	1485.73	J/mol×K	1159.37	Joback Method
cpg	1503.80	J/mol×K	1205.25	Joback Method
cpg	1521.84	J/mol×K	1251.14	Joback Method
cpg	1540.18	J/mol×K	1297.02	Joback Method
cpg	1559.19	J/mol×K	1342.90	Joback Method
cpg	1579.19	J/mol×K	1388.78	Joback Method

Sources

- Cheméo Relay (1.0):
- Cheméo Relay (1.0, beta):
- NIST Webbook:
- Joback Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R438674&Units=SI>

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

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

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

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