

D-(+)-Mannose, pentakis(trifluoroacetate), methyloxime (anti)

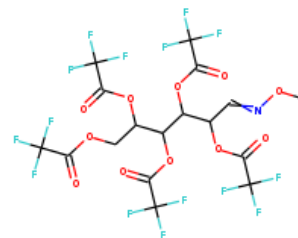
InChI: InChI=1S/C17H10F15NO11/c1-39-33-2-4(41-9(35)14(21,22)23)6(43-11(37)16(27,28)29)7(44-12(38)17(30,31)32)5(42-10(36)15(24,25)26)3-40-8(34)13(18,19)20/h2,4-7H,3H2,1H3

InChI Key: IOALWQFXAPVULK-UHFFFAOYSA-N

Formula: C17H10F15NO11

SMILES: CON=CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F

Molecular Weight: 689.24



Physical Properties

Property	Value	Unit	Source
$\Delta_f H^\circ_{\text{gas}}$	-4674.73	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	84.65	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	2.62		Crippen Method
P_c	923.86	kPa	Joback Method
T_{boil}	1040.05	K	Joback Method
T_c	1307.10	K	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H10F15NO11/c1-39-33-2-4\(41-9\(35\)14\(21,22\)23\)6\(43-11\(37\)16\(27,28\)29\)7\(44-12\(38\)17\(30,31\)32\)5\(42-10\(36\)15\(24,25\)26\)3-40-8\(34\)13\(18,19\)20/h2,4-7H,3H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H10F15NO11/c1-39-33-2-4(41-9(35)14(21,22)23)6(43-11(37)16(27,28)29)7(44-12(38)17(30,31)32)5(42-10(36)15(24,25)26)3-40-8(34)13(18,19)20/h2,4-7H,3H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).
 T_{c} : Critical Temperature (K).

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