BENZALDEHYDE, 3,5-DIMETHOXY-4-[(TRIMETHYLSILYL)OXY]-

Other names: Syringaldehyde, TMS
Syringic aldehyde, TMS
Syringaldehyde, tms derivative

Inchi: InChI=1S/C12H18O4Si/c1-14-10-6-9(8-13)7-11(15-2)12(10)16-17(3,4)5/h6-8H,1-5H3

InchiKey: RYSJAQSTIILRKM-UHFFFAOYSA-N

Formula: C12H18O4Si

SMILES: COc1cc(C=O)cc(OC)c1O[Si](C)(C)C

Mol. weight [g/mol]: 254.36

Physical Properties

Property code	Value	Unit	Source
hvap	73.27	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.31		Cheméo Relay (1.0)
logp	2.730		Crippen Method
tb	570.40	K	Cheméo Relay (1.0)
tf	347.95	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6651623&Units=SI

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

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

Legend

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point

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