tert-Butyldimethylsilyl pentyl phthalate

Other names: 1,2-Benzenedicarboxylic acid, pentyl tert-butyldimethylsilyl ester
Inchi: InChI=1S/C19H30O4Si/c1-7-8-11-14-22-17(20)15-12-9-10-13-16(15)18(21)23-24(5,6)19
InchiKey: MQUBFYXVDVAYJY-UHFFFAOYSA-N
Formula: C19H30O4Si
SMILES: CCCCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 350.52

Physical Properties

Property code	Value	Unit	Source
af	0.8431		Cheméo Relay (1.0)
hf	-899.19	kJ/mol	Cheméo Relay (1.0)
hvap	81.17	kJ/mol	Cheméo Relay (1.0)
log10ws	-4.95		Cheméo Relay (1.0)
logp	5.196		Crippen Method
pc	1261.62	kPa	Cheméo Relay (1.0, beta)
rinpol	2154.00		NIST Webbook
tb	609.22	K	Cheméo Relay (1.0)
tc	831.79	K	Cheméo Relay (1.0)
tf	271.71	K	Cheméo Relay (1.0)
vc	1.083	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373662&Units=SI
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):

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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