(+)-«gamma»-Tocopherol, O-methyl-

Inchi: InChI=1S/C29H50O2/c1-21(2)12-9-13-22(3)14-10-15-23(4)16-11-18-29(7)19-17-26-20-2
InchiKey: YCYZEPRIDWTCRQ-UHFFFAOYSA-N
Formula: C29H50O2
SMILES: COc1cc2c(c(C)c1C)OC(C)(CCCC(C)CCCC(C)CCCC(C)C)CC2
Mol. weight [g/mol]: 430.71

Physical Properties

Property code	Value	Unit	Source
hfus	51.69	kJ/mol	Joback Method
logp	8.835		Crippen Method
mcvol	396.590	ml/mol	McGowan Method
rinpol	2979.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1391.28	J/mol×K	968.82	Joback Method
cpg	1416.83	J/mol×K	1005.13	Joback Method
cpg	1441.82	J/mol×K	1041.44	Joback Method
cpg	1466.42	J/mol×K	1077.75	Joback Method
cpg	1490.77	J/mol×K	1114.06	Joback Method
cpg	1515.05	J/mol×K	1150.37	Joback Method
cpg	1539.41	J/mol×K	1186.68	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374722&Units=SI
Joback Method: 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