3,5-DIETHOXYCARBONYL-2,4,6-TRIMETHYLPYRI

Other names: 3,5-Diethoxycarbonyl-2,4,6-trimethylpyridine
Inchi: InChI=1S/C14H19NO4/c1-6-18-13(16)11-8(3)12(14(17)19-7-2)10(5)15-9(11)4/h6-7H2,1-
InchiKey: IJHKOUDBKFONBB-UHFFFAOYSA-N
Formula: C14H19NO4
SMILES: CCOC(=O)c1c(C)nc(C)c(C(=O)OCC)c1C
Mol. weight [g/mol]: 265.31

Physical Properties

Property code	Value	Unit	Source
af	0.7680		Cheméo Relay (1.0)
hf	-701.73	kJ/mol	Cheméo Relay (1.0)
hvap	76.89	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	2.360		Crippen Method
mcvol	209.220	ml/mol	McGowan Method
pc	1697.24	kPa	Cheméo Relay (1.0, beta)
tb	587.05	K	Cheméo Relay (1.0)
tc	808.78	K	Cheméo Relay (1.0)
tf	346.37	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1150556&Units=SI
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
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point