1,2,3,4-TETRAHYDROISOQUINOLINE, 6,7,8-TRIMETHOXY-1-METHYL-

Other names: Anhalonidine, O-methyl
Inchi: InChI=1S/C13H19NO3/c1-8-11-9(5-6-14-8)7-10(15-2)12(16-3)13(11)17-4/h7-8,14H,5-6H
InchiKey: VMFUYWSNWQYUTG-UHFFFAOYSA-N
Formula: C13H19NO3
SMILES: COc1cc2c(c(OC)c1OC)C(C)NCC2
Mol. weight [g/mol]: 237.30

Physical Properties

Property code	Value	Unit	Source
hfus	31.10	kJ/mol	Joback Method
logp	1.919		Crippen Method
mcvol	187.000	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.60	J/mol×K	670.26	Joback Method
cpg	526.55	J/mol×K	706.73	Joback Method
cpg	542.58	J/mol×K	743.19	Joback Method
cpg	557.65	J/mol×K	779.66	Joback Method
cpg	571.76	J/mol×K	816.12	Joback Method
cpg	584.88	J/mol×K	852.59	Joback Method
cpg	597.00	J/mol×K	889.05	Joback Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U127935&Units=SI

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

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume