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]: 237.29

Physical Properties

Property code	Value	Unit	Source
gf	-46.17	kJ/mol	Joback Method
hf	-413.21	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.919		Crippen Method
mcvol	187.000	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
tb	670.26	K	Joback Method
tc	889.05	K	Joback Method
tf	498.91	K	Joback Method
vc	0.696	m3/kmol	Joback 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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U127935&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
vc:	Critical Volume