Anhalinine

Other names: 1,2,3,4-Tetrahydroquinoline, 6,7,8-trimethoxy-
Inchi: InChI=1S/C12H17NO3/c1-14-10-6-8-4-5-13-7-9(8)11(15-2)12(10)16-3/h6,13H,4-5,7H2,1
InchiKey: GOBKARNYNSWQFZ-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: COc1cc2c(c(OC)c1OC)CNCC2
Mol. weight [g/mol]: 223.27
CAS: 642-30-8

Physical Properties

Property code	Value	Unit	Source
gf	-46.88	kJ/mol	Joback Method
hf	-372.23	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.358		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	652.05	K	Joback Method
tc	874.69	K	Joback Method
tf	491.88	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.17	J/mol×K	652.05	Joback Method
cpg	471.11	J/mol×K	689.16	Joback Method
cpg	486.18	J/mol×K	726.26	Joback Method
cpg	500.37	J/mol×K	763.37	Joback Method
cpg	513.67	J/mol×K	800.48	Joback Method
cpg	526.06	J/mol×K	837.58	Joback Method
cpg	537.53	J/mol×K	874.69	Joback Method

Sources

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=C642308&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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