1,3-Dioxolo[4,5-h]isoquinoline, 6,7,8,9-tetrahydro-4-methoxy-9-methyl-, (S)-

Other names: Anhalonine
Inchi: InChI=1S/C12H15NO3/c1-7-10-8(3-4-13-7)5-9(14-2)11-12(10)16-6-15-11/h5,7,13H,3-4,6
InchiKey: YEGBVDVRKMCCON-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: COc1cc2c(c3c1OCO3)C(C)NCC2
Mol. weight [g/mol]: 221.25
CAS: 519-04-0

Physical Properties

Property code	Value	Unit	Source
gf	51.63	kJ/mol	Joback Method
hf	-298.99	kJ/mol	Joback Method
hfus	39.16	kJ/mol	Joback Method
hvap	65.72	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	1.631		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
rinpol	1850.00		NIST Webbook
tb	667.85	K	Joback Method
tc	906.52	K	Joback Method
tf	518.50	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.85	J/mol×K	667.85	Joback Method
cpg	464.44	J/mol×K	707.63	Joback Method
cpg	478.99	J/mol×K	747.41	Joback Method
cpg	492.58	J/mol×K	787.19	Joback Method
cpg	505.25	J/mol×K	826.96	Joback Method
cpg	517.06	J/mol×K	866.74	Joback Method
cpg	528.07	J/mol×K	906.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C519040&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume