Anhalonidine

Inchi: InChI=1S/C12H17NO3/c1-7-10-8(4-5-13-7)6-9(15-2)12(16-3)11(10)14/h6-7,13-14H,4-5H
InchiKey: PRNZAMQMBOFSJY-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: COc1cc2c(c(O)c1OC)C(C)NCC2
Mol. weight [g/mol]: 223.27
CAS: 17627-77-9

Physical Properties

Property code	Value	Unit	Source
gf	-94.58	kJ/mol	Joback Method
hf	-426.19	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.616		Crippen Method
mcvol	172.910	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
rinpol	1825.00		NIST Webbook
tb	700.60	K	Joback Method
tc	933.64	K	Joback Method
tf	564.61	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.23	J/mol×K	700.60	Joback Method
cpg	501.40	J/mol×K	739.44	Joback Method
cpg	515.69	J/mol×K	778.28	Joback Method
cpg	529.15	J/mol×K	817.12	Joback Method
cpg	541.84	J/mol×K	855.96	Joback Method
cpg	553.80	J/mol×K	894.80	Joback Method
cpg	565.08	J/mol×K	933.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17627779&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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