4-ALLYL-5-AMINO VERATROLE

Other names: 2-Allyl-4,5-dimethoxyaniline
Inchi: InChI=1S/C11H15NO2/c1-4-5-8-6-10(13-2)11(14-3)7-9(8)12/h4,6-7H,1,5,12H2,2-3H3
InchiKey: HFEJTRNCHBWDOQ-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: C=CCc1cc(OC)c(OC)cc1N
Mol. weight [g/mol]: 193.25

Physical Properties

Property code	Value	Unit	Source
hfus	23.41	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	2.014		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	584.04	K	Cheméo Relay (1.0)
tf	337.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.27	J/mol×K	606.75	Joback Method
cpg	404.99	J/mol×K	642.54	Joback Method
cpg	418.02	J/mol×K	678.34	Joback Method
cpg	430.36	J/mol×K	714.13	Joback Method
cpg	442.00	J/mol×K	749.93	Joback Method
cpg	452.94	J/mol×K	785.72	Joback Method
cpg	463.18	J/mol×K	821.52	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=C30058516&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point