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]: 193.24
CAS: 30058-51-6

Physical Properties

Property code	Value	Unit	Source
gf	69.55	kJ/mol	Joback Method
hf	-173.47	kJ/mol	Joback Method
hfus	23.41	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.014		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	606.75	K	Joback Method
tc	821.52	K	Joback Method
tf	403.67	K	Joback Method
vc	0.590	m3/kmol	Joback Method

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

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=C30058516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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