Plicatin B

Inchi: InChI=1S/C15H18O3/c1-11(2)4-7-13-10-12(5-8-14(13)16)6-9-15(17)18-3/h4-6,8-10,16H,
InchiKey: LZEOAWXRNGQEHO-RMKNXTFCSA-N
Formula: C15H18O3
SMILES: COC(=O)C=Cc1ccc(O)c(CC=C(C)C)c1
Mol. weight [g/mol]: 246.30

Physical Properties

Property code	Value	Unit	Source
gf	-58.45	kJ/mol	Joback Method
hf	-325.33	kJ/mol	Joback Method
hfus	35.92	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.087		Crippen Method
mcvol	203.160	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	2163.00		NIST Webbook
tb	739.37	K	Joback Method
tc	964.78	K	Joback Method
tf	457.51	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.34	J/mol×K	739.37	Joback Method
cpg	569.35	J/mol×K	776.94	Joback Method
cpg	582.58	J/mol×K	814.51	Joback Method
cpg	595.14	J/mol×K	852.08	Joback Method
cpg	607.14	J/mol×K	889.64	Joback Method
cpg	618.68	J/mol×K	927.21	Joback Method
cpg	629.87	J/mol×K	964.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519778&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