4-(2-Propenyl)-phenylangelate

Inchi: InChI=1S/C14H16O2/c1-4-6-12-7-9-13(10-8-12)16-14(15)11(3)5-2/h4-5,7-10H,1,6H2,2-3
InchiKey: MFVAGPYVXQOKCL-WZUFQYTHSA-N
Formula: C14H16O2
SMILES: C=CCc1ccc(OC(=O)C(C)=CC)cc1
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	95.37	kJ/mol	Joback Method
hf	-119.17	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.287		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
ripol	2252.00		NIST Webbook
ripol	2252.00		NIST Webbook
tb	628.39	K	Joback Method
tc	844.96	K	Joback Method
tf	337.84	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.76	J/mol×K	628.39	Joback Method
cpg	466.01	J/mol×K	664.49	Joback Method
cpg	480.31	J/mol×K	700.58	Joback Method
cpg	493.70	J/mol×K	736.68	Joback Method
cpg	506.23	J/mol×K	772.77	Joback Method
cpg	517.95	J/mol×K	808.87	Joback Method
cpg	528.89	J/mol×K	844.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R514124&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume