Orcinyl angelate

Inchi: InChI=1S/C12H14O3/c1-4-9(3)12(14)15-11-6-8(2)5-10(13)7-11/h4-7,13H,1-3H3/b9-4-
InchiKey: AFRZSDNGGFCOLA-WTKPLQERSA-N
Formula: C12H14O3
SMILES: CC=C(C)C(=O)Oc1cc(C)cc(O)c1
Mol. weight [g/mol]: 206.24

Physical Properties

Property code	Value	Unit	Source
gf	-163.93	kJ/mol	Joback Method
hf	-380.63	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.572		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
ripol	2767.00		NIST Webbook
ripol	2767.00		NIST Webbook
tb	666.57	K	Joback Method
tc	895.59	K	Joback Method
tf	428.78	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.33	J/mol×K	666.57	Joback Method
cpg	437.20	J/mol×K	704.74	Joback Method
cpg	449.27	J/mol×K	742.91	Joback Method
cpg	460.61	J/mol×K	781.08	Joback Method
cpg	471.32	J/mol×K	819.25	Joback Method
cpg	481.48	J/mol×K	857.42	Joback Method
cpg	491.17	J/mol×K	895.59	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R639382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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