Avenaciolide, 6-(2-phenylethyl)

Inchi: InChI=1S/C15H14O4/c1-9-12-11(8-7-10-5-3-2-4-6-10)18-15(17)13(12)19-14(9)16/h2-6,1
InchiKey: WBDYUBHQOBHZGQ-JHJVBQTASA-N
Formula: C15H14O4
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3ccccc3)C12
Mol. weight [g/mol]: 258.27

Physical Properties

Property code	Value	Unit	Source
gf	-86.92	kJ/mol	Joback Method
hf	-458.62	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	68.79	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.642		Crippen Method
mcvol	187.310	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	775.33	K	Joback Method
tc	1028.42	K	Joback Method
tf	513.09	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.19	J/mol×K	775.33	Joback Method
cpg	594.91	J/mol×K	817.51	Joback Method
cpg	610.10	J/mol×K	859.69	Joback Method
cpg	623.77	J/mol×K	901.87	Joback Method
cpg	635.93	J/mol×K	944.06	Joback Method
cpg	646.59	J/mol×K	986.24	Joback Method
cpg	655.78	J/mol×K	1028.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565885&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume