Avenaciolide, 6-[2-(4-methylphenyl)ethyl]-4-demethylene

Inchi: InChI=1S/C15H16O4/c1-9-2-4-10(5-3-9)6-7-12-11-8-13(16)19-14(11)15(17)18-12/h2-5,1

InchiKey: JKERMARNKVNMQC-YRGRVCCFSA-N

Formula: C15H16O4

SMILES: Cc1ccc(CCC2OC(=O)C3OC(=O)CC23)cc1

Mol. weight [g/mol]: 260.29

Physical Properties

Property code	Value	Unit	Source
gf	-149.63	kJ/mol	Joback Method
hf	-554.33	kJ/mol	Joback Method
hfus	36.38	kJ/mol	Joback Method
hvap	69.30	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.785		Crippen Method
mcvol	191.610	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	2300.00		NIST Webbook
tb	781.15	K	Joback Method
tc	1033.01	K	Joback Method
tf	511.93	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.45	J/mol×K	781.15	Joback Method
cpg	621.95	J/mol×K	823.13	Joback Method
cpg	637.88	J/mol×K	865.10	Joback Method
cpg	652.26	J/mol×K	907.08	Joback Method
cpg	665.09	J/mol×K	949.05	Joback Method
cpg	676.40	J/mol×K	991.03	Joback Method
cpg	686.20	J/mol×K	1033.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565850&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