Avenaciolide, 1-dihydro-6-(2-phenylethyl)-4-demethylene

Inchi: InChI=1S/C14H16O4/c15-13-9-8-12(18-14(16)10-17-13)7-6-11-4-2-1-3-5-11/h1-5,12H,6-

InchiKey: HPTMZEXRPOEIKD-GFCCVEGCSA-N

Formula: C14H16O4

SMILES: O=C1CCC(CCc2ccccc2)OC(=O)CO1

Mol. weight [g/mol]: 248.27

Physical Properties

Property code	Value	Unit	Source
gf	-237.76	kJ/mol	Joback Method
hf	-593.16	kJ/mol	Joback Method
hfus	28.67	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.868		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	764.03	K	Joback Method
tc	1027.65	K	Joback Method
tf	463.88	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.38	J/mol×K	764.03	Joback Method
cpg	591.13	J/mol×K	807.97	Joback Method
cpg	607.89	J/mol×K	851.90	Joback Method
cpg	622.61	J/mol×K	895.84	Joback Method
cpg	635.23	J/mol×K	939.78	Joback Method
cpg	645.69	J/mol×K	983.71	Joback Method
cpg	653.94	J/mol×K	1027.65	Joback Method

Sources

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=R565716&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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