Avenaciolide, 1-dihydro-6-[2-(4-methylphenyl)ethyl]-4-demethyl

Inchi: InChI=1S/C15H18O4/c1-11-2-4-12(5-3-11)6-7-13-8-9-14(16)18-10-15(17)19-13/h2-5,13H

InchiKey: MJJDYPXFUCBUEY-CYBMUJFWSA-N

Formula: C15H18O4

SMILES: Cc1ccc(CCC2CCC(=O)OCC(=O)O2)cc1

Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-238.97	kJ/mol	Joback Method
hf	-625.27	kJ/mol	Joback Method
hfus	30.87	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.176		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	791.89	K	Joback Method
tc	1050.24	K	Joback Method
tf	487.67	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.48	J/mol×K	791.89	Joback Method
cpg	645.95	J/mol×K	834.95	Joback Method
cpg	662.41	J/mol×K	878.01	Joback Method
cpg	676.79	J/mol×K	921.07	Joback Method
cpg	689.04	J/mol×K	964.13	Joback Method
cpg	699.08	J/mol×K	1007.18	Joback Method
cpg	706.87	J/mol×K	1050.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565692&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