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

Inchi: InChI=1S/C14H13FO4/c15-9-4-1-8(2-5-9)3-6-11-10-7-12(16)19-13(10)14(17)18-11/h1-2,

InchiKey: WVJZOHTUQCJUSD-NQBHXWOUSA-N

Formula: C14H13FO4

SMILES: O=C1CC2C(CCc3ccc(F)cc3)OC(=O)C2O1

Mol. weight [g/mol]: 264.25

Physical Properties

Property code	Value	Unit	Source
gf	-352.86	kJ/mol	Joback Method
hf	-729.80	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	66.25	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.615		Crippen Method
mcvol	179.290	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	2230.00		NIST Webbook
tb	757.54	K	Joback Method
tc	1003.76	K	Joback Method
tf	501.25	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.93	J/mol×K	757.54	Joback Method
cpg	573.47	J/mol×K	798.58	Joback Method
cpg	588.58	J/mol×K	839.61	Joback Method
cpg	602.27	J/mol×K	880.65	Joback Method
cpg	614.54	J/mol×K	921.68	Joback Method
cpg	625.42	J/mol×K	962.72	Joback Method
cpg	634.91	J/mol×K	1003.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565830&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

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