Avenaciolide, 1-dihydro-6-[2-(4-fluorophenyl)ethyl]-4-demethyle

Inchi: InChI=1S/C14H15FO4/c15-11-4-1-10(2-5-11)3-6-12-7-8-13(16)18-9-14(17)19-12/h1-2,4-

InchiKey: UKIULMNSSNQUCF-GFCCVEGCSA-N

Formula: C14H15FO4

SMILES: O=C1CCC(CCc2ccc(F)cc2)OC(=O)CO1

Mol. weight [g/mol]: 266.26

Physical Properties

Property code	Value	Unit	Source
gf	-442.20	kJ/mol	Joback Method
hf	-800.74	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	67.17	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.007		Crippen Method
mcvol	190.150	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2165.00		NIST Webbook
tb	768.28	K	Joback Method
tc	1020.98	K	Joback Method
tf	476.99	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.16	J/mol×K	768.28	Joback Method
cpg	596.83	J/mol×K	810.40	Joback Method
cpg	612.68	J/mol×K	852.51	Joback Method
cpg	626.66	J/mol×K	894.63	Joback Method
cpg	638.71	J/mol×K	936.75	Joback Method
cpg	648.77	J/mol×K	978.86	Joback Method
cpg	656.77	J/mol×K	1020.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565687&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