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

Inchi: InChI=1S/C16H16O4/c1-9-3-5-11(6-4-9)7-8-12-13-10(2)15(17)20-14(13)16(18)19-12/h3-
InchiKey: ZMMUVXIZTSCXCJ-MGPQQGTHSA-N
Formula: C16H16O4
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3ccc(C)cc3)C12
Mol. weight [g/mol]: 272.30

Physical Properties

Property code	Value	Unit	Source
gf	-88.13	kJ/mol	Joback Method
hf	-490.73	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	1.951		Crippen Method
mcvol	201.400	ml/mol	McGowan Method
pc	2289.32	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	803.19	K	Joback Method
tc	1051.81	K	Joback Method
tf	536.88	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.74	J/mol×K	803.19	Joback Method
cpg	649.43	J/mol×K	844.63	Joback Method
cpg	664.57	J/mol×K	886.06	Joback Method
cpg	678.17	J/mol×K	927.50	Joback Method
cpg	690.25	J/mol×K	968.93	Joback Method
cpg	700.80	J/mol×K	1010.37	Joback Method
cpg	709.84	J/mol×K	1051.81	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=R565845&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