Avenaciolide, 6-[2-(3-ethoxyphenyl)ethyl]

Inchi: InChI=1S/C17H18O5/c1-3-20-12-6-4-5-11(9-12)7-8-13-14-10(2)16(18)22-15(14)17(19)21
InchiKey: ZFSCAQFLODEVQR-RBSFLKMASA-N
Formula: C17H18O5
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3cccc(OCC)c3)C12
Mol. weight [g/mol]: 302.32

Physical Properties

Property code	Value	Unit	Source
gf	-184.71	kJ/mol	Joback Method
hf	-643.59	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.041		Crippen Method
mcvol	221.360	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	2553.00		NIST Webbook
tb	848.49	K	Joback Method
tc	1089.46	K	Joback Method
tf	570.38	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.02	J/mol×K	848.49	Joback Method
cpg	732.90	J/mol×K	888.65	Joback Method
cpg	747.16	J/mol×K	928.81	Joback Method
cpg	759.77	J/mol×K	968.97	Joback Method
cpg	770.74	J/mol×K	1009.13	Joback Method
cpg	780.05	J/mol×K	1049.29	Joback Method
cpg	787.70	J/mol×K	1089.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565781&Units=SI

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