Avenaciolide, 1-dihydro-6-[2-(3-ethoxyphenyl)ethyl]-4-demethyl

Inchi: InChI=1S/C16H20O5/c1-2-19-14-5-3-4-12(10-14)6-7-13-8-9-15(17)20-11-16(18)21-13/h3

InchiKey: QQARBWOMLWEZRU-CYBMUJFWSA-N

Formula: C16H20O5

SMILES: CCOc1cccc(CCC2CCC(=O)OCC(=O)O2)c1

Mol. weight [g/mol]: 292.33

Physical Properties

Property code	Value	Unit	Source
gf	-335.55	kJ/mol	Joback Method
hf	-778.13	kJ/mol	Joback Method
hfus	34.65	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	2.267		Crippen Method
mcvol	222.430	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	837.19	K	Joback Method
tc	1086.38	K	Joback Method
tf	521.17	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.57	J/mol×K	837.19	Joback Method
cpg	729.80	J/mol×K	878.72	Joback Method
cpg	744.89	J/mol×K	920.25	Joback Method
cpg	757.79	J/mol×K	961.78	Joback Method
cpg	768.42	J/mol×K	1003.32	Joback Method
cpg	776.70	J/mol×K	1044.85	Joback Method
cpg	782.56	J/mol×K	1086.38	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=R565667&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