Avenaciolide, 6-[2-(2-chlorophenyl)ethyl]

Inchi: InChI=1S/C15H13ClO4/c1-8-12-11(19-15(18)13(12)20-14(8)17)7-6-9-4-2-3-5-10(9)16/h2
InchiKey: YQJDSRFDYQPDOX-JHJVBQTASA-N
Formula: C15H13ClO4
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3ccccc3Cl)C12
Mol. weight [g/mol]: 292.71

Physical Properties

Property code	Value	Unit	Source
gf	-108.48	kJ/mol	Joback Method
hf	-485.83	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	73.84	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.296		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2395.00		NIST Webbook
tb	817.74	K	Joback Method
tc	1073.21	K	Joback Method
tf	555.53	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.59	J/mol×K	817.74	Joback Method
cpg	616.56	J/mol×K	860.32	Joback Method
cpg	630.01	J/mol×K	902.90	Joback Method
cpg	641.93	J/mol×K	945.48	Joback Method
cpg	652.33	J/mol×K	988.05	Joback Method
cpg	661.23	J/mol×K	1030.63	Joback Method
cpg	668.62	J/mol×K	1073.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565721&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