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

Inchi: InChI=1S/C14H15ClO4/c15-12-4-2-1-3-10(12)5-6-11-7-8-13(16)18-9-14(17)19-11/h1-4,1

InchiKey: MJUPTNVLMFWXEF-LLVKDONJSA-N

Formula: C14H15ClO4

SMILES: O=C1CCC(CCc2ccccc2Cl)OC(=O)CO1

Mol. weight [g/mol]: 282.72

Physical Properties

Property code	Value	Unit	Source
gf	-259.32	kJ/mol	Joback Method
hf	-620.37	kJ/mol	Joback Method
hfus	32.48	kJ/mol	Joback Method
hvap	72.37	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.521		Crippen Method
mcvol	200.620	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	806.44	K	Joback Method
tc	1072.12	K	Joback Method
tf	506.32	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.19	J/mol×K	806.44	Joback Method
cpg	613.79	J/mol×K	850.72	Joback Method
cpg	628.34	J/mol×K	895.00	Joback Method
cpg	640.77	J/mol×K	939.28	Joback Method
cpg	651.01	J/mol×K	983.56	Joback Method
cpg	659.00	J/mol×K	1027.84	Joback Method
cpg	664.67	J/mol×K	1072.12	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=R565632&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

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