Avenaciolide, 6-[2-(3-chlorophenyl)ethyl]-4-demethylene

Inchi: InChI=1S/C14H13ClO4/c15-9-3-1-2-8(6-9)4-5-11-10-7-12(16)19-13(10)14(17)18-11/h1-3

InchiKey: PKAZUMWPTJAWHC-NQBHXWOUSA-N

Formula: C14H13ClO4

SMILES: O=C1CC2C(CCc3cccc(Cl)c3)OC(=O)C2O1

Mol. weight [g/mol]: 280.70

Physical Properties

Property code	Value	Unit	Source
gf	-169.98	kJ/mol	Joback Method
hf	-549.43	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	71.46	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.130		Crippen Method
mcvol	189.760	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	2435.00		NIST Webbook
tb	795.70	K	Joback Method
tc	1054.74	K	Joback Method
tf	530.58	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.36	J/mol×K	795.70	Joback Method
cpg	590.12	J/mol×K	838.87	Joback Method
cpg	604.32	J/mol×K	882.05	Joback Method
cpg	616.98	J/mol×K	925.22	Joback Method
cpg	628.11	J/mol×K	968.39	Joback Method
cpg	637.73	J/mol×K	1011.56	Joback Method
cpg	645.86	J/mol×K	1054.74	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=R565776&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

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