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

Inchi: InChI=1S/C14H13BrO4/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: HLCOJZCLLLCBOV-NQBHXWOUSA-N

Formula: C14H13BrO4

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

Mol. weight [g/mol]: 325.15

Physical Properties

Property code	Value	Unit	Source
gf	-143.73	kJ/mol	Joback Method
hf	-507.36	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	73.51	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.239		Crippen Method
mcvol	195.020	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	2540.00		NIST Webbook
tb	824.43	K	Joback Method
tc	1090.81	K	Joback Method
tf	560.46	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.61	J/mol×K	824.43	Joback Method
cpg	600.68	J/mol×K	868.83	Joback Method
cpg	614.17	J/mol×K	913.22	Joback Method
cpg	626.12	J/mol×K	957.62	Joback Method
cpg	636.54	J/mol×K	1002.02	Joback Method
cpg	645.48	J/mol×K	1046.41	Joback Method
cpg	652.96	J/mol×K	1090.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565756&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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