Avenaciolide, 1-dihydro-6-[2-(3-bromophenyl)ethyl]-4-demethyle

Inchi: InChI=1S/C14H15BrO4/c15-11-3-1-2-10(8-11)4-5-12-6-7-13(16)18-9-14(17)19-12/h1-3,8

InchiKey: LOOMUFOPWHDJNZ-GFCCVEGCSA-N

Formula: C14H15BrO4

SMILES: O=C1CCC(CCc2cccc(Br)c2)OC(=O)CO1

Mol. weight [g/mol]: 327.17

Physical Properties

Property code	Value	Unit	Source
gf	-233.07	kJ/mol	Joback Method
hf	-578.30	kJ/mol	Joback Method
hfus	33.57	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	2.630		Crippen Method
mcvol	205.880	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	2464.00		NIST Webbook
tb	835.17	K	Joback Method
tc	1108.23	K	Joback Method
tf	536.20	K	Joback Method
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.76	J/mol×K	835.17	Joback Method
cpg	624.40	J/mol×K	880.68	Joback Method
cpg	637.89	J/mol×K	926.19	Joback Method
cpg	649.17	J/mol×K	971.70	Joback Method
cpg	658.18	J/mol×K	1017.21	Joback Method
cpg	664.86	J/mol×K	1062.72	Joback Method
cpg	669.16	J/mol×K	1108.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565647&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