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

Inchi: InChI=1S/C15H13BrO4/c1-8-12-11(19-15(18)13(12)20-14(8)17)6-5-9-3-2-4-10(16)7-9/h2
InchiKey: PQPPZWZZPBSQJW-JHJVBQTASA-N
Formula: C15H13BrO4
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3cccc(Br)c3)C12
Mol. weight [g/mol]: 337.17

Physical Properties

Property code	Value	Unit	Source
gf	-82.23	kJ/mol	Joback Method
hf	-443.76	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.405		Crippen Method
mcvol	204.810	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	846.47	K	Joback Method
tc	1109.02	K	Joback Method
tf	585.41	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.42	J/mol×K	846.47	Joback Method
cpg	626.71	J/mol×K	890.23	Joback Method
cpg	639.45	J/mol×K	933.99	Joback Method
cpg	650.66	J/mol×K	977.74	Joback Method
cpg	660.36	J/mol×K	1021.50	Joback Method
cpg	668.57	J/mol×K	1065.26	Joback Method
cpg	675.32	J/mol×K	1109.02	Joback Method

Sources

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=R565741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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