Avenaciolide, 6-[2-(4-fluorophenyl)ethyl]

Inchi: InChI=1S/C15H13FO4/c1-8-12-11(19-15(18)13(12)20-14(8)17)7-4-9-2-5-10(16)6-3-9/h2-
InchiKey: GYHSDXXIKHSDMA-JHJVBQTASA-N
Formula: C15H13FO4
SMILES: C=C1C(=O)OC2C(=O)OC(CCc3ccc(F)cc3)C12
Mol. weight [g/mol]: 276.26

Physical Properties

Property code	Value	Unit	Source
gf	-291.36	kJ/mol	Joback Method
hf	-666.20	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	1.781		Crippen Method
mcvol	189.080	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	2244.00		NIST Webbook
rinpol	2244.00		NIST Webbook
tb	779.58	K	Joback Method
tc	1022.75	K	Joback Method
tf	526.20	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.78	J/mol×K	779.58	Joback Method
cpg	600.58	J/mol×K	820.11	Joback Method
cpg	614.97	J/mol×K	860.64	Joback Method
cpg	627.96	J/mol×K	901.17	Joback Method
cpg	639.55	J/mol×K	941.69	Joback Method
cpg	649.75	J/mol×K	982.22	Joback Method
cpg	658.56	J/mol×K	1022.75	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=R565825&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

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