Avenaciolide, 6-[2-(4-trifluoromethylphenyl)ethyl]-4-demethylen

Inchi: InChI=1S/C15H13F3O4/c16-15(17,18)9-4-1-8(2-5-9)3-6-11-10-7-12(19)22-13(10)14(20)2

InchiKey: VOFVQYNCMZIMJI-NQBHXWOUSA-N

Formula: C15H13F3O4

SMILES: O=C1CC2C(CCc3ccc(C(F)(F)F)cc3)OC(=O)C2O1

Mol. weight [g/mol]: 314.26

Physical Properties

Property code	Value	Unit	Source
gf	-731.22	kJ/mol	Joback Method
hf	-1151.41	kJ/mol	Joback Method
hfus	38.20	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.495		Crippen Method
mcvol	196.920	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	2248.00		NIST Webbook
tb	775.73	K	Joback Method
tc	1009.70	K	Joback Method
tf	516.12	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.32	J/mol×K	775.73	Joback Method
cpg	644.97	J/mol×K	814.73	Joback Method
cpg	659.24	J/mol×K	853.72	Joback Method
cpg	672.18	J/mol×K	892.72	Joback Method
cpg	683.84	J/mol×K	931.71	Joback Method
cpg	694.26	J/mol×K	970.71	Joback Method
cpg	703.49	J/mol×K	1009.70	Joback Method

Sources

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=R565870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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