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

Inchi: InChI=1S/C16H13F3O4/c1-8-12-11(22-15(21)13(12)23-14(8)20)7-4-9-2-5-10(6-3-9)16(17

InchiKey: YWLLMCGXMXJIBR-JHJVBQTASA-N

Formula: C16H13F3O4

SMILES: C=C1C(=O)OC2C(=O)OC(CCc3ccc(C(F)(F)F)cc3)C12

Mol. weight [g/mol]: 326.27

Physical Properties

Property code	Value	Unit	Source
gf	-669.72	kJ/mol	Joback Method
hf	-1087.81	kJ/mol	Joback Method
hfus	39.63	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	2.661		Crippen Method
mcvol	206.710	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	2257.00		NIST Webbook
rinpol	2257.00		NIST Webbook
tb	797.77	K	Joback Method
tc	1029.51	K	Joback Method
tf	541.07	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.22	J/mol×K	797.77	Joback Method
cpg	672.14	J/mol×K	836.39	Joback Method
cpg	685.73	J/mol×K	875.02	Joback Method
cpg	698.02	J/mol×K	913.64	Joback Method
cpg	709.05	J/mol×K	952.26	Joback Method
cpg	718.84	J/mol×K	990.88	Joback Method
cpg	727.45	J/mol×K	1029.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R565865&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