4-Methoxy-2-(3-methyloxiranyl)-phenyl angelate

Other names: 4-Methoxy-2-(3-methyloxiranyl)phenyl angelate (=epoxypseudoisoeugenyl angelate)

Inchi: InChI=1S/C15H18O4/c1-5-9(2)15(16)19-13-7-6-11(17-4)8-12(13)14-10(3)18-14/h5-8,10,

InchiKey: SRKAZFSLCLSHPY-UITAMQMPSA-N

Formula: C15H18O4

SMILES: CC=C(C)C(=O)Oc1ccc(OC)cc1C1OC1C

Mol. weight [g/mol]: 262.30

Physical Properties

Property code	Value	Unit	Source
gf	-131.76	kJ/mol	Joback Method
hf	-488.47	kJ/mol	Joback Method
hfus	37.92	kJ/mol	Joback Method
hvap	68.30	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.027		Crippen Method
mcvol	202.470	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
ripol	2825.00		NIST Webbook
ripol	2825.00		NIST Webbook
ripol	2825.00		NIST Webbook
tb	711.01	K	Joback Method
tc	929.75	K	Joback Method
tf	425.89	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.64	J/mol×K	711.01	Joback Method
cpg	585.49	J/mol×K	747.47	Joback Method
cpg	600.34	J/mol×K	783.92	Joback Method
cpg	614.20	J/mol×K	820.38	Joback Method
cpg	627.14	J/mol×K	856.84	Joback Method
cpg	639.18	J/mol×K	893.29	Joback Method

cpg	650.37	J/mol×K	929.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418303&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume