10-Isobutyryloxy-8,9-epoxythymyl angelate

Inchi: InChI=1S/C20H26O5/c1-6-15(5)19(22)25-17-10-14(4)7-8-16(17)20(12-24-20)11-23-18(2
InchiKey: APUXZTFWNUSAOP-UUASQNMZSA-N
Formula: C20H26O5
SMILES: CC=C(C)C(=O)Oc1cc(C)ccc1C1(COC(=O)CC(C)C)CO1
Mol. weight [g/mol]: 346.42

Physical Properties

Property code	Value	Unit	Source
gf	-218.80	kJ/mol	Joback Method
hf	-673.95	kJ/mol	Joback Method
hfus	41.58	kJ/mol	Joback Method
hvap	84.95	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.681		Crippen Method
mcvol	274.490	ml/mol	McGowan Method
pc	1582.23	kPa	Joback Method
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
ripol	2808.00		NIST Webbook
ripol	2808.00		NIST Webbook
tb	883.75	K	Joback Method
tc	1105.58	K	Joback Method
tf	545.31	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.04	J/mol×K	883.75	Joback Method
cpg	880.75	J/mol×K	920.72	Joback Method
cpg	898.14	J/mol×K	957.69	Joback Method
cpg	915.37	J/mol×K	994.66	Joback Method
cpg	932.59	J/mol×K	1031.64	Joback Method
cpg	949.97	J/mol×K	1068.61	Joback Method

cpg	967.65	J/mol×K	1105.58	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=R518280&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume