6-Methoxy 8,9-dehydro-thymyl tiglate

Inchi: InChI=1S/C16H20O3/c1-7-11(4)16(17)19-15-8-12(5)14(18-6)9-13(15)10(2)3/h7-9H,2H2,
InchiKey: GWSRVDBBPMIAMU-YRNVUSSQSA-N
Formula: C16H20O3
SMILES: C=C(C)c1cc(OC)c(C)cc1OC(=O)C(C)=CC
Mol. weight [g/mol]: 260.33

Physical Properties

Property code	Value	Unit	Source
gf	-20.60	kJ/mol	Joback Method
hf	-325.40	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.908		Crippen Method
mcvol	217.250	ml/mol	McGowan Method
pc	1834.11	kPa	Joback Method
rinpol	1867.20		NIST Webbook
rinpol	1867.20		NIST Webbook
tb	706.41	K	Joback Method
tc	918.90	K	Joback Method
tf	393.69	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.61	J/mol×K	706.41	Joback Method
cpg	595.36	J/mol×K	741.82	Joback Method
cpg	610.19	J/mol×K	777.24	Joback Method
cpg	624.11	J/mol×K	812.65	Joback Method
cpg	637.14	J/mol×K	848.07	Joback Method
cpg	649.31	J/mol×K	883.48	Joback Method
cpg	660.64	J/mol×K	918.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413806&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