6-Methoxy thymyl tiglate

Inchi: InChI=1S/C16H22O3/c1-7-11(4)16(17)19-15-8-12(5)14(18-6)9-13(15)10(2)3/h7-10H,1-6
InchiKey: LLEOAKBZOLWGPN-YRNVUSSQSA-N
Formula: C16H22O3
SMILES: CC=C(C)C(=O)Oc1cc(C)c(OC)cc1C(C)C
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-102.33	kJ/mol	Joback Method
hf	-446.32	kJ/mol	Joback Method
hfus	29.41	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.999		Crippen Method
mcvol	221.550	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1859.00		NIST Webbook
rinpol	1859.00		NIST Webbook
tb	709.41	K	Joback Method
tc	918.94	K	Joback Method
tf	394.41	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.48	J/mol×K	709.41	Joback Method
cpg	620.88	J/mol×K	744.33	Joback Method
cpg	636.32	J/mol×K	779.25	Joback Method
cpg	650.82	J/mol×K	814.17	Joback Method
cpg	664.40	J/mol×K	849.10	Joback Method
cpg	677.07	J/mol×K	884.02	Joback Method
cpg	688.85	J/mol×K	918.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U413805&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