8,9-Dehydrothymyl tiglate

Inchi: InChI=1S/C15H18O2/c1-6-12(5)15(16)17-14-9-11(4)7-8-13(14)10(2)3/h6-9H,2H2,1,3-5H
InchiKey: MHVVYWCDJGNGIX-WUXMJOGZSA-N
Formula: C15H18O2
SMILES: C=C(C)c1ccc(C)cc1OC(=O)C(C)=CC
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	85.61	kJ/mol	Joback Method
hf	-161.07	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	61.19	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.900		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1627.00		NIST Webbook
ripol	2205.00		NIST Webbook
tb	656.13	K	Joback Method
tc	873.48	K	Joback Method
tf	347.67	K	Joback Method
vc	0.754	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.81	J/mol×K	656.13	Joback Method
cpg	516.61	J/mol×K	692.35	Joback Method
cpg	531.45	J/mol×K	728.58	Joback Method
cpg	545.38	J/mol×K	764.80	Joback Method
cpg	558.44	J/mol×K	801.03	Joback Method
cpg	570.66	J/mol×K	837.25	Joback Method
cpg	582.10	J/mol×K	873.48	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=R417211&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