Thymyl tiglate

Inchi: InChI=1S/C15H20O2/c1-6-12(5)15(16)17-14-9-11(4)7-8-13(14)10(2)3/h6-10H,1-5H3/b12
InchiKey: UUEIVUJSJLKAAM-WUXMJOGZSA-N
Formula: C15H20O2
SMILES: CC=C(C)C(=O)Oc1cc(C)ccc1C(C)C
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	3.88	kJ/mol	Joback Method
hf	-281.99	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	61.39	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.990		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
ripol	2169.00		NIST Webbook
ripol	2169.00		NIST Webbook
tb	659.13	K	Joback Method
tc	873.07	K	Joback Method
tf	348.39	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.22	J/mol×K	659.13	Joback Method
cpg	540.72	J/mol×K	694.79	Joback Method
cpg	556.26	J/mol×K	730.44	Joback Method
cpg	570.85	J/mol×K	766.10	Joback Method
cpg	584.54	J/mol×K	801.76	Joback Method
cpg	597.36	J/mol×K	837.42	Joback Method

cpg	609.35	J/mol×K	873.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R417291&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
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