Thymyl formate

Inchi: InChI=1S/C11H14O2/c1-8(2)10-5-4-9(3)6-11(10)13-7-12/h4-8H,1-3H3
InchiKey: IWAIRWGSZFYSES-UHFFFAOYSA-N
Formula: C11H14O2
SMILES: Cc1ccc(C(C)C)c(OC=O)c1
Mol. weight [g/mol]: 178.23

Physical Properties

Property code	Value	Unit	Source
gf	-72.07	kJ/mol	Joback Method
hf	-279.86	kJ/mol	Joback Method
hfus	17.46	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.654		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1262.00		NIST Webbook
tb	558.36	K	Joback Method
tc	769.26	K	Joback Method
tf	314.42	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.05	J/mol×K	558.36	Joback Method
cpg	360.93	J/mol×K	593.51	Joback Method
cpg	374.09	J/mol×K	628.66	Joback Method
cpg	386.55	J/mol×K	663.81	Joback Method
cpg	398.32	J/mol×K	698.96	Joback Method
cpg	409.40	J/mol×K	734.11	Joback Method
cpg	419.80	J/mol×K	769.26	Joback Method
dvisc	0.0018829	Pa×s	314.42	Joback Method
dvisc	0.0010402	Pa×s	355.08	Joback Method

dvisc	0.0006491	Pa×s	395.73	Joback Method
dvisc	0.0004423	Pa×s	436.39	Joback Method
dvisc	0.0003217	Pa×s	477.05	Joback Method
dvisc	0.0002460	Pa×s	517.70	Joback Method
dvisc	0.0001956	Pa×s	558.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R590846&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
dvisc:	Dynamic viscosity
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

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