Thymyl isobutyrate

Inchi: InChI=1S/C14H20O2/c1-9(2)12-7-6-11(5)8-13(12)16-14(15)10(3)4/h6-10H,1-5H3
InchiKey: HTPVUEJWIFHSCK-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: Cc1ccc(C(C)C)c(OC(=O)C(C)C)c1
Mol. weight [g/mol]: 220.31
CAS: 5451-67-2

Physical Properties

Property code	Value	Unit	Source
gf	-78.65	kJ/mol	Joback Method
hf	-374.06	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	58.74	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.680		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1480.40		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1480.40		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1889.00		NIST Webbook
ripol	1889.00		NIST Webbook
tb	631.77	K	Joback Method
tc	841.45	K	Joback Method
tf	341.16	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.38	J/mol×K	631.77	Joback Method
cpg	511.02	J/mol×K	666.72	Joback Method
cpg	526.73	J/mol×K	701.66	Joback Method
cpg	541.53	J/mol×K	736.61	Joback Method
cpg	555.44	J/mol×K	771.56	Joback Method
cpg	568.48	J/mol×K	806.51	Joback Method
cpg	580.66	J/mol×K	841.45	Joback Method
dvisc	0.0019087	Pa×s	341.16	Joback Method
dvisc	0.0009197	Pa×s	389.60	Joback Method
dvisc	0.0005208	Pa×s	438.03	Joback Method
dvisc	0.0003303	Pa×s	486.47	Joback Method
dvisc	0.0002275	Pa×s	534.90	Joback Method
dvisc	0.0001667	Pa×s	583.34	Joback Method
dvisc	0.0001281	Pa×s	631.77	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451672&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume