Isothymol isobutyrate

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

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	1500.00		NIST Webbook
rinpol	1500.00		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=R227088&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume