

isothymyl butyrate

Inchi:	InChI=1S/C14H20O2/c1-5-6-14(15)16-13-9-12(10(2)3)8-7-11(13)4/h7-10H,5-6H2,1-4H3
InchiKey:	TUGCSLQMXFBHFI-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CCCC(=O)Oc1cc(C(C)C)ccc1C
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	-76.21	kJ/mol	Joback Method
hf	-368.78	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.824		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
ripol	1907.00		NIST Webbook
ripol	1907.00		NIST Webbook
tb	632.21	K	Joback Method
tc	837.91	K	Joback Method
tf	356.16	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.94	J/mol×K	632.21	Joback Method
cpg	566.69	J/mol×K	803.63	Joback Method
cpg	553.84	J/mol×K	769.34	Joback Method
cpg	540.15	J/mol×K	735.06	Joback Method
cpg	525.62	J/mol×K	700.78	Joback Method
cpg	510.22	J/mol×K	666.49	Joback Method
cpg	578.72	J/mol×K	837.91	Joback Method
dvisc	0.0001377	Pa×s	632.21	Joback Method

dvisc	0.0001757	Pa×s	586.20	Joback Method
dvisc	0.0002338	Pa×s	540.19	Joback Method
dvisc	0.0003281	Pa×s	494.19	Joback Method
dvisc	0.0004935	Pa×s	448.18	Joback Method
dvisc	0.0008151	Pa×s	402.17	Joback Method
dvisc	0.0015325	Pa×s	356.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R522739&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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