

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001757	Paxs	586.20	Joback Method
dvisc	0.0002338	Paxs	540.19	Joback Method
dvisc	0.0003281	Paxs	494.19	Joback Method
dvisc	0.0004935	Paxs	448.18	Joback Method
dvisc	0.0008151	Paxs	402.17	Joback Method
dvisc	0.0015325	Paxs	356.16	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=R522739&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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