

# Italicen-12-yl 2-methylbutyrate

<b>Inchi:</b>	InChI=1S/C20H32O2/c1-6-14(3)18(21)22-12-19(5)16-8-7-15(4)20(16)10-9-13(2)11-17(19)
<b>InchiKey:</b>	UBHUQRYYLLGBFL-XEOZSPBDSA-N
<b>Formula:</b>	C20H32O2
<b>SMILES:</b>	CCC(C)C(=O)OCC1(C)C2C=C(C)CCC23C(C)CCC13
<b>Mol. weight [g/mol]:</b>	304.47

## Physical Properties

Property code	Value	Unit	Source
gf	33.14	kJ/mol	Joback Method
hf	-464.02	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.984		Crippen Method
mvol	263.220	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	2012.00		NIST Webbook
rinpol	2012.00		NIST Webbook
tb	756.89	K	Joback Method
tc	972.13	K	Joback Method
tf	471.70	K	Joback Method
vc	1.008	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.97	J/molxK	756.89	Joback Method
cpg	865.76	J/molxK	792.76	Joback Method
cpg	888.05	J/molxK	828.64	Joback Method
cpg	910.10	J/molxK	864.51	Joback Method
cpg	932.16	J/molxK	900.39	Joback Method
cpg	954.49	J/molxK	936.26	Joback Method
cpg	977.34	J/molxK	972.13	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R233157&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R233157&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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