

# Fragranyl isobutyrate

<b>Inchi:</b>	InChI=1S/C14H24O2/c1-10(2)12-6-7-14(12,5)8-9-16-13(15)11(3)4/h11-12H,1,6-9H2,2-5H1
<b>InchiKey:</b>	FVDDHXILHJBLOF-UHFFFAOYSA-N
<b>Formula:</b>	C14H24O2
<b>SMILES:</b>	<chem>C=C(C)C1CCC1(C)CCOC(=O)C(C)C</chem>
<b>Mol. weight [g/mol]:</b>	224.34
<b>CAS:</b>	51117-23-8

## Physical Properties

Property code	Value	Unit	Source
gf	-54.62	kJ/mol	Joback Method
hf	-405.19	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.568		Crippen Method
mcvol	200.400	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1483.90		NIST Webbook
rinpol	1483.90		NIST Webbook
tb	598.71	K	Joback Method
tc	797.86	K	Joback Method
tf	323.06	K	Joback Method
vc	0.765	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.19	J/molxK	598.71	Joback Method
cpg	551.82	J/molxK	631.90	Joback Method
cpg	569.50	J/molxK	665.09	Joback Method
cpg	586.31	J/molxK	698.28	Joback Method
cpg	602.36	J/molxK	731.48	Joback Method
cpg	617.75	J/molxK	764.67	Joback Method
cpg	632.57	J/molxK	797.86	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=C51117238&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51117238&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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