

# Methyl tropate

<b>Inchi:</b>	InChI=1S/C10H12O3/c1-13-10(12)9(7-11)8-5-3-2-4-6-8/h2-6,9,11H,7H2,1H3
<b>InchiKey:</b>	OLEWRQVKIUHEJP-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O3
<b>SMILES:</b>	COC(=O)C(CO)c1ccccc1
<b>Mol. weight [g/mol]:</b>	180.20
<b>CAS:</b>	3967-53-1

## Physical Properties

Property code	Value	Unit	Source
gf	-227.45	kJ/mol	Joback Method
hf	-415.51	kJ/mol	Joback Method
hfus	19.05	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	0.935		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1429.50		NIST Webbook
rinpol	1418.40		NIST Webbook
tb	622.91	K	Joback Method
tc	825.20	K	Joback Method
tf	346.86	K	Joback Method
vc	0.524	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.77	J/molxK	622.91	Joback Method
cpg	363.16	J/molxK	656.63	Joback Method
cpg	373.87	J/molxK	690.34	Joback Method
cpg	383.91	J/molxK	724.06	Joback Method
cpg	393.31	J/molxK	757.77	Joback Method
cpg	402.07	J/molxK	791.49	Joback Method
cpg	410.23	J/molxK	825.20	Joback Method

dvisc	0.0050139	Paxs	346.86	Joback Method
dvisc	0.0015849	Paxs	392.87	Joback Method
dvisc	0.0006378	Paxs	438.88	Joback Method
dvisc	0.0003051	Paxs	484.88	Joback Method
dvisc	0.0001658	Paxs	530.89	Joback Method
dvisc	0.0000993	Paxs	576.90	Joback Method
dvisc	0.0000642	Paxs	622.91	Joback Method

## Sources

<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=C3967531&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3967531&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hvap:</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>rinpol:</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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