

# Tangerinal I

Inchi:	InChI=1S/C12H22O/c1-2-3-4-5-6-7-8-9-10-11-12-13/h8-9,12H,2-7,10-11H2,1H3
InchiKey:	MMCD SVCBSAMNPL-UHFFFAOYSA-N
Formula:	C12H22O
SMILES:	CCCCCCCC=CCCC=O
Mol. weight [g/mol]:	182.30

## Physical Properties

Property code	Value	Unit	Source
gf	30.86	kJ/mol	Joback Method
hf	-259.37	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	48.98	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.882		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1985.89	kPa	Joback Method
rinpol	1543.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	526.78	K	Joback Method
tc	700.00	K	Joback Method
tf	261.92	K	Joback Method
vc	0.705	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.84	J/molxK	526.78	Joback Method
cpg	488.73	J/molxK	671.13	Joback Method
cpg	476.02	J/molxK	642.26	Joback Method
cpg	462.70	J/molxK	613.39	Joback Method
cpg	448.75	J/molxK	584.52	Joback Method
cpg	434.14	J/molxK	555.65	Joback Method
cpg	500.86	J/molxK	700.00	Joback Method

dvisc	0.0002140	Paxs	526.78	Joback Method
dvisc	0.0002830	Paxs	482.64	Joback Method
dvisc	0.0003959	Paxs	438.49	Joback Method
dvisc	0.0005970	Paxs	394.35	Joback Method
dvisc	0.0009985	Paxs	350.21	Joback Method
dvisc	0.0019373	Paxs	306.06	Joback Method
dvisc	0.0046993	Paxs	261.92	Joback Method

## Sources

<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>
<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=R410245&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R410245&amp;Units=SI</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>ripol:</b>	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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