

# Farnasal

<b>Inchi:</b>	InChI=1S/C15H30O/c1-13(2)7-5-8-14(3)9-6-10-15(4)11-12-16/h12-15H,5-11H2,1-4H3
<b>InchiKey:</b>	BTCKFZHMWUFBQY-UHFFFAOYSA-N
<b>Formula:</b>	C15H30O
<b>SMILES:</b>	CC(C)CCCC(C)CCCC(C)CC=O
<b>Mol. weight [g/mol]:</b>	226.40

## Physical Properties

Property code	Value	Unit	Source
gf	-31.42	kJ/mol	Joback Method
hf	-454.35	kJ/mol	Joback Method
hfus	26.33	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.844		Crippen Method
mvol	223.780	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	589.94	K	Joback Method
tc	762.12	K	Joback Method
tf	255.81	K	Joback Method
vc	0.875	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.96	J/mol×K	589.94	Joback Method
cpg	674.91	J/mol×K	733.42	Joback Method
cpg	659.64	J/mol×K	704.72	Joback Method
cpg	643.64	J/mol×K	676.03	Joback Method
cpg	626.87	J/mol×K	647.33	Joback Method
cpg	609.32	J/mol×K	618.64	Joback Method
cpg	689.46	J/mol×K	762.12	Joback Method
dvisc	0.0001567	Paxs	589.94	Joback Method

dvisc	0.0002242	Paxs	534.25	Joback Method
dvisc	0.0003488	Paxs	478.56	Joback Method
dvisc	0.0006096	Paxs	422.88	Joback Method
dvisc	0.0012620	Paxs	367.19	Joback Method
dvisc	0.0033890	Paxs	311.50	Joback Method
dvisc	0.0139918	Paxs	255.81	Joback Method

## Sources

<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=R574493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R574493&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>

## 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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