

# Galaxolide-I

<b>Inchi:</b>	InChI=1S/C18H26O/c1-11-9-19-10-13-7-15-16(8-14(11)13)18(5,6)12(2)17(15,3)4/h7-8,1
<b>InchiKey:</b>	ONKNPOPIGWHAQC-PIJUOVFKSA-N
<b>Formula:</b>	C18H26O
<b>SMILES:</b>	CC1COCCc2cc3c(cc21)C(C)(C)C(C)C3(C)C
<b>Mol. weight [g/mol]:</b>	258.40

## Physical Properties

Property code	Value	Unit	Source
gf	181.08	kJ/mol	Joback Method
hf	-215.49	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	61.51	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.525		Crippen Method
mvol	224.870	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
ripol	2345.00		NIST Webbook
ripol	2345.00		NIST Webbook
tb	688.70	K	Joback Method
tc	920.33	K	Joback Method
tf	454.85	K	Joback Method
vc	0.857	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.21	J/mol×K	688.70	Joback Method
cpg	681.77	J/mol×K	727.30	Joback Method
cpg	702.55	J/mol×K	765.91	Joback Method
cpg	722.86	J/mol×K	804.51	Joback Method
cpg	742.99	J/mol×K	843.12	Joback Method
cpg	763.23	J/mol×K	881.72	Joback Method
cpg	783.89	J/mol×K	920.33	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=R631011&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R631011&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>
<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>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>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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