

# Bakerol

<b>Inchi:</b>	InChI=1S/C14H24O2/c1-9-5-6-11-12(3,4)16-14(15)10(2)7-8-13(9,11)14/h9-11,15H,5-8H2
<b>InchiKey:</b>	GRRIYLFQXHZWQR-SSYGJKRZSA-N
<b>Formula:</b>	C14H24O2
<b>SMILES:</b>	CC1CCC23C(C)CCC2C(C)(C)OC13O
<b>Mol. weight [g/mol]:</b>	224.34

## Physical Properties

Property code	Value	Unit	Source
gf	-37.49	kJ/mol	Joback Method
hf	-425.74	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.946		Crippen Method
mcvol	187.280	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	654.32	K	Joback Method
tc	869.18	K	Joback Method
tf	440.69	K	Joback Method
vc	0.706	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.67	J/mol×K	654.32	Joback Method
cpg	594.47	J/mol×K	690.13	Joback Method
cpg	612.60	J/mol×K	725.94	Joback Method
cpg	630.39	J/mol×K	761.75	Joback Method
cpg	648.18	J/mol×K	797.56	Joback Method
cpg	666.29	J/mol×K	833.37	Joback Method
cpg	685.06	J/mol×K	869.18	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=R641380&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R641380&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>hvp:</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>rlnol:</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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