

# sedanolide

<b>Other names:</b>	(3S,3aR)-(-)-Sedanolide trans-Sedanolide trans-Neocnidilide Sedanolide, trans- 1(3H)-Isobenzofuranone, 3-butyl-3a,4,5,6-tetrahydro-, (3S,3aR)- Neocnidilide
<b>Inchi:</b>	InChI=1S/C12H18O2/c1-2-3-8-11-9-6-4-5-7-10(9)12(13)14-11/h7,9,11H,2-6,8H2,1H3
<b>InchiKey:</b>	UPJFTVFLSIQQAV-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O2
<b>SMILES:</b>	CCCCC1OC(=O)C2=CCCCC21
<b>Mol. weight [g/mol]:</b>	194.27
<b>CAS:</b>	6415-59-4

## Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-387.28	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.828		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
ripol	1726.00		NIST Webbook
ripol	1735.00		NIST Webbook
ripol	2618.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2550.00		NIST Webbook
tb	599.16	K	Joback Method
tc	822.08	K	Joback Method
tf	358.39	K	Joback Method
vc	0.612	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.41	J/molxK	599.16	Joback Method
cpg	456.37	J/molxK	636.31	Joback Method
cpg	474.21	J/molxK	673.47	Joback Method
cpg	490.96	J/molxK	710.62	Joback Method
cpg	506.65	J/molxK	747.77	Joback Method
cpg	521.32	J/molxK	784.93	Joback Method
cpg	534.98	J/molxK	822.08	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=C4567333&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4567333&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>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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