

# Sebacic acid, isohexyl 2-nitrophenyl ester

<b>Inchi:</b>	InChI=1S/C22H33NO6/c1-18(2)12-11-17-28-21(24)15-7-5-3-4-6-8-16-22(25)29-20-14-10
<b>InchiKey:</b>	AUVDUIDXTBEPGW-UHFFFAOYSA-N
<b>Formula:</b>	C22H33NO6
<b>SMILES:</b>	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1ccccc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	407.50

## Physical Properties

Property code	Value	Unit	Source
gf	-197.59	kJ/mol	Joback Method
hf	-777.99	kJ/mol	Joback Method
hfus	59.80	kJ/mol	Joback Method
hvap	102.02	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.600		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
rinsol	3107.00		NIST Webbook
tb	1038.40	K	Joback Method
tc	1271.66	K	Joback Method
tf	649.57	K	Joback Method
vc	1.284	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.70	J/molxK	1038.40	Joback Method
cpg	1121.45	J/molxK	1077.28	Joback Method
cpg	1132.70	J/molxK	1116.15	Joback Method
cpg	1142.50	J/molxK	1155.03	Joback Method
cpg	1150.89	J/molxK	1193.90	Joback Method
cpg	1157.93	J/molxK	1232.78	Joback Method
cpg	1163.67	J/molxK	1271.66	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=U354797&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354797&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>

# 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>hvac:</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>mccol:</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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