

# Sebacic acid, ethyl 4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C19H27NO6/c1-2-25-18(21)9-7-5-3-4-6-8-10-19(22)26-15-16-11-13-17(14-12-
<b>InchiKey:</b>	GFDDGNOYIBIWKV-UHFFFAOYSA-N
<b>Formula:</b>	C19H27NO6
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)OCc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	365.42

## Physical Properties

Property code	Value	Unit	Source
gf	-220.41	kJ/mol	Joback Method
hf	-710.79	kJ/mol	Joback Method
hfus	55.55	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.322		Crippen Method
mvol	287.110	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	970.20	K	Joback Method
tc	1193.92	K	Joback Method
tf	630.76	K	Joback Method
vc	1.121	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.17	J/mol×K	970.20	Joback Method
cpg	941.66	J/mol×K	1007.49	Joback Method
cpg	952.85	J/mol×K	1044.77	Joback Method
cpg	962.77	J/mol×K	1082.06	Joback Method
cpg	971.45	J/mol×K	1119.34	Joback Method
cpg	978.94	J/mol×K	1156.63	Joback Method
cpg	985.26	J/mol×K	1193.92	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=U380802&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380802&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.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>rinpola:</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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