

# Sebacic acid, ethyl 3-methoxy-4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C20H29NO7/c1-3-27-19(22)10-8-6-4-5-7-9-11-20(23)28-15-16-12-13-17(21)(24)
<b>InchiKey:</b>	RUICCFHXEWCEGL-UHFFFAOYSA-N
<b>Formula:</b>	C20H29NO7
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)OCc1ccc([N+](=O)[O-])c(OC)c1
<b>Mol. weight [g/mol]:</b>	395.45

## Physical Properties

Property code	Value	Unit	Source
gf	-326.62	kJ/mol	Joback Method
hf	-875.12	kJ/mol	Joback Method
hfus	58.94	kJ/mol	Joback Method
hvap	101.03	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.330		Crippen Method
mvol	307.070	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	3017.00		NIST Webbook
rinpol	3017.00		NIST Webbook
tb	1020.48	K	Joback Method
tc	1250.53	K	Joback Method
tf	676.78	K	Joback Method
vc	1.196	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.05	J/molxK	1020.48	Joback Method
cpg	1024.45	J/molxK	1058.82	Joback Method
cpg	1034.24	J/molxK	1097.16	Joback Method
cpg	1042.45	J/molxK	1135.50	Joback Method
cpg	1049.10	J/molxK	1173.85	Joback Method
cpg	1054.19	J/molxK	1212.19	Joback Method
cpg	1057.73	J/molxK	1250.53	Joback Method

# Sources

<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=U380801&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380801&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>

# 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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