

# Sebacic acid, but-3-enyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C20H36O4/c1-4-5-16-23-19(21)14-10-8-6-7-9-11-15-20(22)24-17-12-13-18(2)3
<b>InchiKey:</b>	WZPJASHKSZBULY-UHFFFAOYSA-N
<b>Formula:</b>	C20H36O4
<b>SMILES:</b>	C=CCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	340.50

## Physical Properties

Property code	Value	Unit	Source
gf	-264.92	kJ/mol	Joback Method
hf	-825.58	kJ/mol	Joback Method
hfus	48.33	kJ/mol	Joback Method
hvap	77.37	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.206		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
rinpol	2337.00		NIST Webbook
tb	805.82	K	Joback Method
tc	990.69	K	Joback Method
tf	442.72	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.73	J/molxK	805.82	Joback Method
cpg	1021.64	J/molxK	959.88	Joback Method
cpg	1007.82	J/molxK	929.06	Joback Method
cpg	993.04	J/molxK	898.25	Joback Method
cpg	977.28	J/molxK	867.44	Joback Method
cpg	960.52	J/molxK	836.63	Joback Method
cpg	1034.51	J/molxK	990.69	Joback Method
dvisc	0.0000522	Paxs	805.82	Joback Method
dvisc	0.0000700	Paxs	745.30	Joback Method

dvisc	0.0000987	Paxs	684.79	Joback Method
dvisc	0.0001489	Paxs	624.27	Joback Method
dvisc	0.0002452	Paxs	563.75	Joback Method
dvisc	0.0004555	Paxs	503.24	Joback Method
dvisc	0.0010021	Paxs	442.72	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=U356085&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356085&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>dvisc:</b>	Dynamic viscosity
<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>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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