

# Sebacic acid, heptyl 3-methylbut-2-enyl ester

<b>Inchi:</b>	InChI=1S/C22H40O4/c1-4-5-6-11-14-18-25-21(23)15-12-9-7-8-10-13-16-22(24)26-19-17
<b>InchiKey:</b>	HZTXVCIVIQHSER-UHFFFAOYSA-N
<b>Formula:</b>	C22H40O4
<b>SMILES:</b>	CCCCCCCOC(=O)CCCCCCCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	368.55

## Physical Properties

Property code	Value	Unit	Source
gf	-261.81	kJ/mol	Joback Method
hf	-879.58	kJ/mol	Joback Method
hfus	57.20	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.130		Crippen Method
mvol	331.420	ml/mol	McGowan Method
pc	988.26	kPa	Joback Method
rinpol	2591.00		NIST Webbook
tb	859.38	K	Joback Method
tc	1052.77	K	Joback Method
tf	462.98	K	Joback Method
vc	1.296	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.44	J/mol×K	859.38	Joback Method
cpg	1084.03	J/mol×K	891.61	Joback Method
cpg	1101.49	J/mol×K	923.84	Joback Method
cpg	1117.88	J/mol×K	956.08	Joback Method
cpg	1133.21	J/mol×K	988.31	Joback Method
cpg	1147.52	J/mol×K	1020.54	Joback Method
cpg	1160.85	J/mol×K	1052.77	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U355880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355880&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</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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