

# Sebacic acid, hex-4-yn-3-yl isobutyl ester

<b>Inchi:</b>	InChI=1S/C20H34O4/c1-5-13-18(6-2)24-20(22)15-12-10-8-7-9-11-14-19(21)23-16-17(3)
<b>InchiKey:</b>	RKVQQXFRTCAJIJ-UHFFFAOYSA-N
<b>Formula:</b>	C20H34O4
<b>SMILES:</b>	CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	338.48

## Physical Properties

Property code	Value	Unit	Source
gf	-152.40	kJ/mol	Joback Method
hf	-683.99	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.652		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpola	2299.00		NIST Webbook
tb	817.70	K	Joback Method
tc	1011.28	K	Joback Method
tf	535.58	K	Joback Method
vc	1.153	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.80	J/molxK	817.70	Joback Method
cpg	938.39	J/molxK	849.96	Joback Method
cpg	954.89	J/molxK	882.23	Joback Method
cpg	970.32	J/molxK	914.49	Joback Method
cpg	984.69	J/molxK	946.75	Joback Method
cpg	998.02	J/molxK	979.02	Joback Method
cpg	1010.33	J/molxK	1011.28	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=U355821&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355821&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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