

# Sebacic acid, 6-ethyloct-3-yl isobutyl ester

<b>Inchi:</b>	InChI=1S/C24H46O4/c1-6-21(7-2)17-18-22(8-3)28-24(26)16-14-12-10-9-11-13-15-23(25)
<b>InchiKey:</b>	CAAVLDDSPKWRNQ-UHFFFAOYSA-N
<b>Formula:</b>	C24H46O4
<b>SMILES:</b>	CCC(CC)CCC(CC)OC(=O)CCCCCCCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	398.62

## Physical Properties

Property code	Value	Unit	Source
gf	-323.96	kJ/mol	Joback Method
hf	-1044.13	kJ/mol	Joback Method
hfus	52.92	kJ/mol	Joback Method
hvap	86.17	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.845		Crippen Method
mvol	363.900	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	2613.00		NIST Webbook
rinpol	2613.00		NIST Webbook
tb	899.78	K	Joback Method
tc	1101.76	K	Joback Method
tf	459.56	K	Joback Method
vc	1.409	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.83	J/molxK	899.78	Joback Method
cpg	1238.81	J/molxK	933.44	Joback Method
cpg	1257.37	J/molxK	967.11	Joback Method
cpg	1274.54	J/molxK	1000.77	Joback Method
cpg	1290.36	J/molxK	1034.43	Joback Method
cpg	1304.87	J/molxK	1068.10	Joback Method
cpg	1318.09	J/molxK	1101.76	Joback Method
dvisc	0.0008558	Paxs	459.56	Joback Method

dvisc	0.0003072	Paxs	532.93	Joback Method
dvisc	0.0001413	Paxs	606.30	Joback Method
dvisc	0.0000768	Paxs	679.67	Joback Method
dvisc	0.0000471	Paxs	753.04	Joback Method
dvisc	0.0000314	Paxs	826.41	Joback Method
dvisc	0.0000224	Paxs	899.78	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354183&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354183&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>

## 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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