

# Sebacic acid, isobutyl 2-isopropylphenyl ester

<b>Inchi:</b>	InChI=1S/C23H36O4/c1-18(2)17-26-22(24)15-9-7-5-6-8-10-16-23(25)27-21-14-12-11-13
<b>InchiKey:</b>	NOKSMQVBKLZKIW-UHFFFAOYSA-N
<b>Formula:</b>	C23H36O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCCCCC(=O)Oc1ccccc1C(C)C
<b>Mol. weight [g/mol]:</b>	376.53

## Physical Properties

Property code	Value	Unit	Source
gf	-227.16	kJ/mol	Joback Method
hf	-793.15	kJ/mol	Joback Method
hfus	47.51	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.035		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpola	2678.00		NIST Webbook
tb	909.00	K	Joback Method
tc	1116.60	K	Joback Method
tf	502.23	K	Joback Method
vc	1.252	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.99	J/molxK	909.00	Joback Method
cpg	1130.24	J/molxK	1082.00	Joback Method
cpg	1118.53	J/molxK	1047.40	Joback Method
cpg	1105.58	J/molxK	1012.80	Joback Method
cpg	1091.36	J/molxK	978.20	Joback Method
cpg	1075.84	J/molxK	943.60	Joback Method
cpg	1140.75	J/molxK	1116.60	Joback Method
dvisc	0.0000298	Paxs	909.00	Joback Method
dvisc	0.0000398	Paxs	841.20	Joback Method

dvisc	0.0000559	Paxs	773.41	Joback Method
dvisc	0.0000840	Paxs	705.61	Joback Method
dvisc	0.0001374	Paxs	637.82	Joback Method
dvisc	0.0002529	Paxs	570.02	Joback Method
dvisc	0.0005486	Paxs	502.23	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=U354828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354828&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>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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