

# Sebacic acid, 3-chlorophenyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C20H29ClO4/c1-16(2)15-24-19(22)12-7-5-3-4-6-8-13-20(23)25-18-11-9-10-17
<b>InchiKey:</b>	GXPUARNZWJETAN-UHFFFAOYSA-N
<b>Formula:</b>	C20H29ClO4
<b>SMILES:</b>	CC(C)COC(=O)CCCCCCCCC(=O)Oc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	368.89

## Physical Properties

Property code	Value	Unit	Source
gf	-261.91	kJ/mol	Joback Method
hf	-741.69	kJ/mol	Joback Method
hfus	47.46	kJ/mol	Joback Method
hvap	85.36	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.565		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinqol	2701.00		NIST Webbook
tb	878.23	K	Joback Method
tc	1085.09	K	Joback Method
tf	513.34	K	Joback Method
vc	1.139	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.47	J/molxK	878.23	Joback Method
cpg	920.52	J/molxK	912.71	Joback Method
cpg	934.40	J/molxK	947.18	Joback Method
cpg	947.12	J/molxK	981.66	Joback Method
cpg	958.72	J/molxK	1016.14	Joback Method
cpg	969.21	J/molxK	1050.62	Joback Method
cpg	978.64	J/molxK	1085.09	Joback Method
dvisc	0.0005407	Paxs	513.34	Joback Method
dvisc	0.0002839	Paxs	574.15	Joback Method

dvisc	0.0001687	Paxs	634.97	Joback Method
dvisc	0.0001098	Paxs	695.78	Joback Method
dvisc	0.0000765	Paxs	756.60	Joback Method
dvisc	0.0000563	Paxs	817.41	Joback Method
dvisc	0.0000432	Paxs	878.23	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354858&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354858&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>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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