

# Sebacic acid, butyl 4-chloro-3-methylphenyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-3-4-15-25-20(23)11-9-7-5-6-8-10-12-21(24)26-18-13-14-19(22)
InchiKey:	ZVNOEMDQVGGDEV-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	CCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	382.92

## Physical Properties

Property code	Value	Unit	Source
gf	-260.68	kJ/mol	Joback Method
hf	-768.52	kJ/mol	Joback Method
hfus	53.18	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.018		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinqol	2859.00		NIST Webbook
tb	906.53	K	Joback Method
tc	1114.56	K	Joback Method
tf	552.13	K	Joback Method
vc	1.200	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.52	J/molxK	906.53	Joback Method
cpg	1027.05	J/molxK	1079.89	Joback Method
cpg	1016.69	J/molxK	1045.22	Joback Method
cpg	1005.17	J/molxK	1010.55	Joback Method
cpg	992.49	J/molxK	975.87	Joback Method
cpg	978.62	J/molxK	941.20	Joback Method
cpg	1036.30	J/molxK	1114.56	Joback Method
dvisc	0.0000416	Paxs	906.53	Joback Method
dvisc	0.0000529	Paxs	847.46	Joback Method

dvisc	0.0000697	Paxs	788.40	Joback Method
dvisc	0.0000961	Paxs	729.33	Joback Method
dvisc	0.0001402	Paxs	670.26	Joback Method
dvisc	0.0002201	Paxs	611.20	Joback Method
dvisc	0.0003804	Paxs	552.13	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354845&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354845&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>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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