

# Sebacic acid, isobutyl 2,4,6-trichlorobenzyl ester

<b>Inchi:</b>	InChI=1S/C21H29Cl3O4/c1-15(2)13-27-20(25)9-7-5-3-4-6-8-10-21(26)28-14-17-18(23)1
<b>InchiKey:</b>	LQUIBOVJZSBXJR-UHFFFAOYSA-N
<b>Formula:</b>	C21H29Cl3O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCCCCCC(=O)OCc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	451.81

## Physical Properties

Property code	Value	Unit	Source
gf	-296.61	kJ/mol	Joback Method
hf	-816.75	kJ/mol	Joback Method
hfus	57.66	kJ/mol	Joback Method
hvap	97.68	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	7.010		Crippen Method
mcvol	334.590	ml/mol	McGowan Method
pc	1142.12	kPa	Joback Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	985.93	K	Joback Method
tc	1208.79	K	Joback Method
tf	609.49	K	Joback Method
vc	1.292	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.56	J/molxK	985.93	Joback Method
cpg	1023.13	J/molxK	1023.07	Joback Method
cpg	1034.38	J/molxK	1060.22	Joback Method
cpg	1044.32	J/molxK	1097.36	Joback Method
cpg	1052.98	J/molxK	1134.50	Joback Method
cpg	1060.39	J/molxK	1171.64	Joback Method
cpg	1066.58	J/molxK	1208.79	Joback Method
dvisc	0.0002412	Paxs	609.49	Joback Method

dvisc	0.0001421	Paxs	672.23	Joback Method
dvisc	0.0000916	Paxs	734.97	Joback Method
dvisc	0.0000633	Paxs	797.71	Joback Method
dvisc	0.0000462	Paxs	860.45	Joback Method
dvisc	0.0000351	Paxs	923.19	Joback Method
dvisc	0.0000277	Paxs	985.93	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=U380573&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380573&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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