

# Sebacic acid, butyl 2,5-dichlorobenzyl ester

<b>Inchi:</b>	InChI=1S/C21H30Cl2O4/c1-2-3-14-26-20(24)10-8-6-4-5-7-9-11-21(25)27-16-17-15-18(2
<b>InchiKey:</b>	ILTUTXLKUAQRNI-UHFFFAOYSA-N
<b>Formula:</b>	C21H30Cl2O4
<b>SMILES:</b>	CCCCOC(=O)CCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	417.37

## Physical Properties

Property code	Value	Unit	Source
gf	-272.61	kJ/mol	Joback Method
hf	-784.26	kJ/mol	Joback Method
hfus	57.38	kJ/mol	Joback Method
hvap	93.02	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.501		Crippen Method
mvol	322.350	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2913.00		NIST Webbook
rinpol	2913.00		NIST Webbook
tb	943.96	K	Joback Method
tc	1158.36	K	Joback Method
tf	582.05	K	Joback Method
vc	1.250	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.45	J/molxK	943.96	Joback Method
cpg	1002.36	J/molxK	979.69	Joback Method
cpg	1015.03	J/molxK	1015.43	Joback Method
cpg	1026.47	J/molxK	1051.16	Joback Method
cpg	1036.72	J/molxK	1086.89	Joback Method
cpg	1045.81	J/molxK	1122.62	Joback Method
cpg	1053.76	J/molxK	1158.36	Joback Method
dvisc	0.0003100	Paxs	582.05	Joback Method

dvisc	0.0001821	Paxs	642.37	Joback Method
dvisc	0.0001172	Paxs	702.69	Joback Method
dvisc	0.0000809	Paxs	763.00	Joback Method
dvisc	0.0000589	Paxs	823.32	Joback Method
dvisc	0.0000448	Paxs	883.64	Joback Method
dvisc	0.0000353	Paxs	943.96	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380613&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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