

# Sebacic acid, 2,5-dichlorobenzyl ethyl ester

<b>Inchi:</b>	InChI=1S/C19H26Cl2O4/c1-2-24-18(22)9-7-5-3-4-6-8-10-19(23)25-14-15-13-16(20)11-12
<b>InchiKey:</b>	GLRUNMAKVXUWCK-UHFFFAOYSA-N
<b>Formula:</b>	C19H26Cl2O4
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)OCc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	389.31

## Physical Properties

Property code	Value	Unit	Source
gf	-289.45	kJ/mol	Joback Method
hf	-742.98	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.720		Crippen Method
mvol	294.170	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	898.20	K	Joback Method
tc	1108.62	K	Joback Method
tf	559.51	K	Joback Method
vc	1.137	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.45	J/molxK	898.20	Joback Method
cpg	883.95	J/molxK	933.27	Joback Method
cpg	896.32	J/molxK	968.34	Joback Method
cpg	907.58	J/molxK	1003.41	Joback Method
cpg	917.74	J/molxK	1038.48	Joback Method
cpg	926.82	J/molxK	1073.55	Joback Method
cpg	934.86	J/molxK	1108.62	Joback Method
dvisc	0.0003863	Paxs	559.51	Joback Method

dvisc	0.0002321	Paxs	615.96	Joback Method
dvisc	0.0001519	Paxs	672.41	Joback Method
dvisc	0.0001062	Paxs	728.86	Joback Method
dvisc	0.0000781	Paxs	785.30	Joback Method
dvisc	0.0000599	Paxs	841.75	Joback Method
dvisc	0.0000475	Paxs	898.20	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380610&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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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