

# Sebacic acid, butyl 2,4-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C20H28Cl2O4/c1-2-3-14-25-19(23)10-8-6-4-5-7-9-11-20(24)26-18-13-12-16(2
<b>InchiKey:</b>	PHIBKKKUJIMODU-UHFFFAOYSA-N
<b>Formula:</b>	C20H28Cl2O4
<b>SMILES:</b>	CCCCOC(=O)CCCCCCCC(=O)Oc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	403.34

## Physical Properties

Property code	Value	Unit	Source
gf	-281.03	kJ/mol	Joback Method
hf	-763.62	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.363		Crippen Method
mcvol	308.260	ml/mol	McGowan Method
pc	1258.37	kPa	Joback Method
rinqol	2873.00		NIST Webbook
tb	921.08	K	Joback Method
tc	1133.06	K	Joback Method
tf	570.78	K	Joback Method
vc	1.194	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.13	J/molxK	921.08	Joback Method
cpg	942.84	J/molxK	956.41	Joback Method
cpg	955.36	J/molxK	991.74	Joback Method
cpg	966.72	J/molxK	1027.07	Joback Method
cpg	976.94	J/molxK	1062.40	Joback Method
cpg	986.04	J/molxK	1097.73	Joback Method
cpg	994.05	J/molxK	1133.06	Joback Method
dvisc	0.0003466	Paxs	570.78	Joback Method
dvisc	0.0002059	Paxs	629.16	Joback Method

dvisc	0.0001336	Paxs	687.55	Joback Method
dvisc	0.0000928	Paxs	745.93	Joback Method
dvisc	0.0000679	Paxs	804.31	Joback Method
dvisc	0.0000519	Paxs	862.70	Joback Method
dvisc	0.0000410	Paxs	921.08	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=U354568&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354568&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>

## 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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