

# Sebacic acid, 4-chloro-2-methylbenzyl decyl ester

Inchi:	InChI=1S/C28H45ClO4/c1-3-4-5-6-7-10-13-16-21-32-27(30)17-14-11-8-9-12-15-18-28(3
InchiKey:	RPWCRSYOQNORGQ-UHFFFAOYSA-N
Formula:	C28H45ClO4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)OCc1ccc(Cl)cc1C
Mol. weight [g/mol]:	481.11

## Physical Properties

Property code	Value	Unit	Source
gf	-201.74	kJ/mol	Joback Method
hf	-913.00	kJ/mol	Joback Method
hfus	71.31	kJ/mol	Joback Method
hvap	104.22	kJ/mol	Joback Method
log10ws	-9.61		Crippen Method
logp	8.496		Crippen Method
mvol	408.740	ml/mol	McGowan Method
pc	793.49	kPa	Joback Method
rinpol	3472.00		NIST Webbook
rinpol	3472.00		NIST Webbook
tb	1066.69	K	Joback Method
tc	1314.62	K	Joback Method
tf	631.02	K	Joback Method
vc	1.593	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.04	J/molxK	1066.69	Joback Method
cpg	1459.92	J/molxK	1273.30	Joback Method
cpg	1450.28	J/molxK	1231.98	Joback Method
cpg	1438.95	J/molxK	1190.66	Joback Method
cpg	1425.85	J/molxK	1149.33	Joback Method
cpg	1410.91	J/molxK	1108.01	Joback Method
cpg	1467.94	J/molxK	1314.62	Joback Method
dvisc	0.0000143	Paxs	1066.69	Joback Method

dvisc	0.0000186	Paxs	994.08	Joback Method
dvisc	0.0000251	Paxs	921.47	Joback Method
dvisc	0.0000356	Paxs	848.86	Joback Method
dvisc	0.0000541	Paxs	776.24	Joback Method
dvisc	0.0000895	Paxs	703.63	Joback Method
dvisc	0.0001662	Paxs	631.02	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U380592&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380592&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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