

# Sebacic acid, 3,5-dichlorophenyl heptyl ester

<b>Inchi:</b>	InChI=1S/C23H34Cl2O4/c1-2-3-4-9-12-15-28-22(26)13-10-7-5-6-8-11-14-23(27)29-21-1
<b>InchiKey:</b>	NJUXXHXBEWOKBI-UHFFFAOYSA-N
<b>Formula:</b>	C23H34Cl2O4
<b>SMILES:</b>	CCCCCCCC(=O)CCCCCCCC(=O)Oc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	445.42

## Physical Properties

Property code	Value	Unit	Source
gf	-255.77	kJ/mol	Joback Method
hf	-825.54	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.533		Crippen Method
mvol	350.530	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	989.72	K	Joback Method
tc	1211.74	K	Joback Method
tf	604.59	K	Joback Method
vc	1.361	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.77	J/molxK	989.72	Joback Method
cpg	1166.86	J/molxK	1174.74	Joback Method
cpg	1157.88	J/molxK	1137.74	Joback Method
cpg	1147.62	J/molxK	1100.73	Joback Method
cpg	1136.04	J/molxK	1063.73	Joback Method
cpg	1123.10	J/molxK	1026.72	Joback Method
cpg	1174.60	J/molxK	1211.74	Joback Method
dvisc	0.0000260	Paxs	989.72	Joback Method

dvisc	0.0000333	Paxs	925.53	Joback Method
dvisc	0.0000440	Paxs	861.34	Joback Method
dvisc	0.0000610	Paxs	797.15	Joback Method
dvisc	0.0000895	Paxs	732.97	Joback Method
dvisc	0.0001412	Paxs	668.78	Joback Method
dvisc	0.0002456	Paxs	604.59	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=U355279&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355279&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>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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