

# Sebacic acid, ethyl 4-formylphenyl ester

<b>Inchi:</b>	InChI=1S/C19H26O5/c1-2-23-18(21)9-7-5-3-4-6-8-10-19(22)24-17-13-11-16(15-20)12-14
<b>InchiKey:</b>	OYEXBUPZQSIIRG-UHFFFAOYSA-N
<b>Formula:</b>	C19H26O5
<b>SMILES:</b>	CCOC(=O)CCCCCCCC(=O)Oc1ccc(C=O)cc1
<b>Mol. weight [g/mol]:</b>	334.41

## Physical Properties

Property code	Value	Unit	Source
gf	-355.48	kJ/mol	Joback Method
hf	-785.61	kJ/mol	Joback Method
hfus	46.48	kJ/mol	Joback Method
hvap	85.86	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.088		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2687.00		NIST Webbook
rinpol	2687.00		NIST Webbook
tb	867.02	K	Joback Method
tc	1071.96	K	Joback Method
tf	529.15	K	Joback Method
vc	1.056	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.14	J/mol×K	867.02	Joback Method
cpg	849.23	J/mol×K	901.18	Joback Method
cpg	862.21	J/mol×K	935.33	Joback Method
cpg	874.10	J/mol×K	969.49	Joback Method
cpg	884.91	J/mol×K	1003.65	Joback Method
cpg	894.68	J/mol×K	1037.81	Joback Method
cpg	903.43	J/mol×K	1071.96	Joback Method
dvisc	0.0006244	Paxs	529.15	Joback Method

dvisc	0.0003612	Paxs	585.46	Joback Method
dvisc	0.0002301	Paxs	641.77	Joback Method
dvisc	0.0001576	Paxs	698.09	Joback Method
dvisc	0.0001142	Paxs	754.40	Joback Method
dvisc	0.0000865	Paxs	810.71	Joback Method
dvisc	0.0000680	Paxs	867.02	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U354884&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354884&amp;Units=SI</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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