

# Sebacic acid, ethyl 2-naphthyl ester

Inchi:	InChI=1S/C22H28O4/c1-2-25-21(23)13-7-5-3-4-6-8-14-22(24)26-20-16-15-18-11-9-10-12
InchiKey:	ODTAHMXIURIBSR-UHFFFAOYSA-N
Formula:	C22H28O4
SMILES:	CCOC(=O)CCCCCCCCC(=O)Oc1ccc2ccccc2c1
Mol. weight [g/mol]:	356.46

## Physical Properties

Property code	Value	Unit	Source
gf	-124.05	kJ/mol	Joback Method
hf	-570.88	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	87.46	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.429		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	2994.00		NIST Webbook
tb	905.98	K	Joback Method
tc	1119.89	K	Joback Method
tf	553.66	K	Joback Method
vc	1.129	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.00	J/molxK	905.98	Joback Method
cpg	984.14	J/molxK	1084.24	Joback Method
cpg	973.31	J/molxK	1048.59	Joback Method
cpg	961.53	J/molxK	1012.93	Joback Method
cpg	948.76	J/molxK	977.28	Joback Method
cpg	934.94	J/molxK	941.63	Joback Method
cpg	994.08	J/molxK	1119.89	Joback Method
dvisc	0.0000834	Paxs	905.98	Joback Method
dvisc	0.0001034	Paxs	847.26	Joback Method

dvisc	0.0001322	Paxs	788.54	Joback Method
dvisc	0.0001760	Paxs	729.82	Joback Method
dvisc	0.0002463	Paxs	671.10	Joback Method
dvisc	0.0003677	Paxs	612.38	Joback Method
dvisc	0.0005974	Paxs	553.66	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=U354834&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354834&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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