

# Succinic acid, 2-(adamant-1-yl)ethyl hept-2-yl ester

Inchi:	InChI=1S/C23H38O4/c1-3-4-5-6-17(2)27-22(25)8-7-21(24)26-10-9-23-14-18-11-19(15-23)
InchiKey:	UUXNBSWYDRYVOU-UHFFFAOYSA-N
Formula:	C23H38O4
SMILES:	CCCCC(C)OC(=O)CCC(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	378.55

## Physical Properties

Property code	Value	Unit	Source
gf	-170.55	kJ/mol	Joback Method
hf	-805.79	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.428		Crippen Method
mcvol	317.230	ml/mol	McGowan Method
pc	1189.88	kPa	Joback Method
rinpola	2800.00		NIST Webbook
rinpola	2800.00		NIST Webbook
tb	897.84	K	Joback Method
tc	1107.10	K	Joback Method
tf	548.25	K	Joback Method
vc	1.226	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.76	J/mol×K	897.84	Joback Method
cpg	1134.89	J/mol×K	932.72	Joback Method
cpg	1156.57	J/mol×K	967.59	Joback Method
cpg	1177.99	J/mol×K	1002.47	Joback Method
cpg	1199.30	J/mol×K	1037.35	Joback Method
cpg	1220.69	J/mol×K	1072.22	Joback Method
cpg	1242.32	J/mol×K	1107.10	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=U391366&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391366&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>hvp:</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>rinp:</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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