

# Isophthalic acid, 1-adamantylmethyl nonyl ester

Inchi:	InChI=1S/C28H40O4/c1-2-3-4-5-6-7-8-12-31-26(29)24-10-9-11-25(16-24)27(30)32-20-28
InchiKey:	QOZGXXKUQOHYPP-UHFFFAOYSA-N
Formula:	C28H40O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)c1
Mol. weight [g/mol]:	440.61

## Physical Properties

Property code	Value	Unit	Source
gf	-23.23	kJ/mol	Joback Method
hf	-678.65	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	97.62	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.967		Crippen Method
mvol	363.920	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	4141.00		NIST Webbook
rinpol	4141.00		NIST Webbook
tb	1044.34	K	Joback Method
tc	1279.67	K	Joback Method
tf	658.54	K	Joback Method
vc	1.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.40	J/molxK	1044.34	Joback Method
cpg	1367.11	J/molxK	1083.56	Joback Method
cpg	1393.08	J/molxK	1122.78	Joback Method
cpg	1419.58	J/molxK	1162.00	Joback Method
cpg	1446.87	J/molxK	1201.22	Joback Method
cpg	1475.23	J/molxK	1240.44	Joback Method
cpg	1504.91	J/molxK	1279.67	Joback Method

# Sources

<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=U343969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343969&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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