

# Isophthalic acid, isoheptyl 3-methylbut-2-en-1-yl ester

<b>Inchi:</b>	InChI=1S/C19H26O4/c1-14(2)7-6-11-22-18(20)16-8-5-9-17(13-16)19(21)23-12-10-15(3)
<b>InchiKey:</b>	SDNDULSPKLCURE-UHFFFAOYSA-N
<b>Formula:</b>	C19H26O4
<b>SMILES:</b>	CC(C)=CCOC(=O)c1cccc(C(=O)OCCCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	318.41

## Physical Properties

Property code	Value	Unit	Source
gf	-186.73	kJ/mol	Joback Method
hf	-597.88	kJ/mol	Joback Method
hfus	39.56	kJ/mol	Joback Method
hvap	78.79	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.403		Crippen Method
mvol	265.390	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2399.00		NIST Webbook
tb	821.96	K	Joback Method
tc	1030.51	K	Joback Method
tf	453.11	K	Joback Method
vc	1.014	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.23	J/molxK	821.96	Joback Method
cpg	808.98	J/molxK	856.72	Joback Method
cpg	823.63	J/molxK	891.48	Joback Method
cpg	837.22	J/molxK	926.24	Joback Method
cpg	849.79	J/molxK	960.99	Joback Method
cpg	861.37	J/molxK	995.75	Joback Method
cpg	871.98	J/molxK	1030.51	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=U343937&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U343937&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.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>

# 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>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>rinpola:</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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