

# Isophthalic acid, isoheptyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C23H28O4/c1-16(2)7-6-14-26-22(24)19-8-5-9-20(15-19)23(25)27-21-12-10-18
InchiKey:	DGYHZOVKWIGFLH-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CC(C)CCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1
Mol. weight [g/mol]:	368.47

## Physical Properties

Property code	Value	Unit	Source
gf	-124.38	kJ/mol	Joback Method
hf	-568.09	kJ/mol	Joback Method
hfus	41.16	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.622		Crippen Method
mvol	302.290	ml/mol	McGowan Method
pc	1386.08	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	940.66	K	Joback Method
tc	1167.15	K	Joback Method
tf	541.17	K	Joback Method
vc	1.143	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.88	J/molxK	940.66	Joback Method
cpg	1015.00	J/molxK	1129.40	Joback Method
cpg	1006.09	J/molxK	1091.65	Joback Method
cpg	995.86	J/molxK	1053.90	Joback Method
cpg	984.28	J/molxK	1016.16	Joback Method
cpg	971.30	J/molxK	978.41	Joback Method
cpg	1022.64	J/molxK	1167.15	Joback Method
dvisc	0.0000312	Paxs	940.66	Joback Method

dvisc	0.0000407	Paxs	874.08	Joback Method
dvisc	0.0000553	Paxs	807.50	Joback Method
dvisc	0.0000794	Paxs	740.91	Joback Method
dvisc	0.0001224	Paxs	674.33	Joback Method
dvisc	0.0002076	Paxs	607.75	Joback Method
dvisc	0.0004011	Paxs	541.17	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=U344456&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344456&amp;Units=SI</a>
<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.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>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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