

# Isophthalic acid, 4-isopropylphenyl propyl ester

Inchi:	InChI=1S/C20H22O4/c1-4-12-23-19(21)16-6-5-7-17(13-16)20(22)24-18-10-8-15(9-11-18)
InchiKey:	MFKOZNZDZFJOQF-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CCCOC(=O)c1cccc(C(=O)Oc2ccc(C(C)C)cc2)c1
Mol. weight [g/mol]:	326.39

## Physical Properties

Property code	Value	Unit	Source
gf	-147.20	kJ/mol	Joback Method
hf	-500.89	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.596		Crippen Method
mvol	260.020	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	872.46	K	Joback Method
tc	1099.91	K	Joback Method
tf	522.36	K	Joback Method
vc	0.982	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.90	J/molxK	872.46	Joback Method
cpg	795.15	J/molxK	910.37	Joback Method
cpg	808.06	J/molxK	948.28	Joback Method
cpg	819.68	J/molxK	986.18	Joback Method
cpg	830.02	J/molxK	1024.09	Joback Method
cpg	839.13	J/molxK	1062.00	Joback Method
cpg	847.04	J/molxK	1099.91	Joback Method
dvisc	0.0004963	Paxs	522.36	Joback Method

dvisc	0.0002824	Paxs	580.71	Joback Method
dvisc	0.0001781	Paxs	639.06	Joback Method
dvisc	0.0001213	Paxs	697.41	Joback Method
dvisc	0.0000877	Paxs	755.76	Joback Method
dvisc	0.0000664	Paxs	814.11	Joback Method
dvisc	0.0000522	Paxs	872.46	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=U344452&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U344452&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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