

# Isophthalic acid, 2-ethylphenyl propyl ester

<b>Inchi:</b>	InChI=1S/C19H20O4/c1-3-12-22-18(20)15-9-7-10-16(13-15)19(21)23-17-11-6-5-8-14(17)
<b>InchiKey:</b>	ODNTYISRIPLQKG-UHFFFAOYSA-N
<b>Formula:</b>	C19H20O4
<b>SMILES:</b>	CCCOC(=O)c1cccc(C(=O)Oc2ccccc2CC)c1
<b>Mol. weight [g/mol]:</b>	312.36

## Physical Properties

Property code	Value	Unit	Source
gf	-153.18	kJ/mol	Joback Method
hf	-474.97	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	82.08	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.035		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2395.00		NIST Webbook
tb	850.02	K	Joback Method
tc	1076.64	K	Joback Method
tf	526.09	K	Joback Method
vc	0.931	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.25	J/molxK	850.02	Joback Method
cpg	737.24	J/molxK	887.79	Joback Method
cpg	749.97	J/molxK	925.56	Joback Method
cpg	761.46	J/molxK	963.33	Joback Method
cpg	771.74	J/molxK	1001.10	Joback Method
cpg	780.85	J/molxK	1038.87	Joback Method
cpg	788.81	J/molxK	1076.64	Joback Method
dvisc	0.0004955	Paxs	526.09	Joback Method
dvisc	0.0003019	Paxs	580.08	Joback Method

dvisc	0.0002002	Paxs	634.07	Joback Method
dvisc	0.0001415	Paxs	688.06	Joback Method
dvisc	0.0001053	Paxs	742.04	Joback Method
dvisc	0.0000815	Paxs	796.03	Joback Method
dvisc	0.0000652	Paxs	850.02	Joback Method

## Sources

<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.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=U356760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356760&amp;Units=SI</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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