

# Isophthalic acid, 2-ethylbutyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C29H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-32-28(30)26-20-19-21-
<b>InchiKey:</b>	QKNAURMUWSECJU-UHFFFAOYSA-N
<b>Formula:</b>	C29H48O4
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(CC)CC)c1
<b>Mol. weight [g/mol]:</b>	460.69

## Physical Properties

Property code	Value	Unit	Source
gf	-174.20	kJ/mol	Joback Method
hf	-911.71	kJ/mol	Joback Method
hfus	66.57	kJ/mol	Joback Method
hvap	101.01	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.528		Crippen Method
mvol	410.590	ml/mol	McGowan Method
pc	777.64	kPa	Joback Method
rinpol	3317.00		NIST Webbook
rinpol	3317.00		NIST Webbook
tb	1046.72	K	Joback Method
tc	1288.88	K	Joback Method
tf	584.85	K	Joback Method
vc	1.593	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1433.30	J/molxK	1046.72	Joback Method
cpg	1451.71	J/molxK	1087.08	Joback Method
cpg	1468.21	J/molxK	1127.44	Joback Method
cpg	1482.86	J/molxK	1167.80	Joback Method
cpg	1495.77	J/molxK	1208.16	Joback Method
cpg	1507.00	J/molxK	1248.52	Joback Method
cpg	1516.63	J/molxK	1288.88	Joback Method
dvisc	0.0002283	Paxs	584.85	Joback Method

dvisc	0.0001073	Paxs	661.83	Joback Method
dvisc	0.0000590	Paxs	738.81	Joback Method
dvisc	0.0000363	Paxs	815.78	Joback Method
dvisc	0.0000243	Paxs	892.76	Joback Method
dvisc	0.0000173	Paxs	969.74	Joback Method
dvisc	0.0000130	Paxs	1046.72	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356435&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356435&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.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>

## 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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