

# Isobutyric acid, 3-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C12H16O2/c1-4-10-6-5-7-11(8-10)14-12(13)9(2)3/h5-9H,4H2,1-3H3
<b>InchiKey:</b>	WZYZFPRBCJHKOI-UHFFFAOYSA-N
<b>Formula:</b>	C12H16O2
<b>SMILES:</b>	CCc1cccc(OC(=O)C(C)C)c1
<b>Mol. weight [g/mol]:</b>	192.25

## Physical Properties

Property code	Value	Unit	Source
gf	-83.42	kJ/mol	Joback Method
hf	-316.03	kJ/mol	Joback Method
hfus	19.75	kJ/mol	Joback Method
hvap	54.01	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.810		Crippen Method
mvol	163.620	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1420.00		NIST Webbook
tb	581.47	K	Joback Method
tc	792.78	K	Joback Method
tf	321.10	K	Joback Method
vc	0.618	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.16	J/molxK	581.47	Joback Method
cpg	409.45	J/molxK	616.69	Joback Method
cpg	423.89	J/molxK	651.91	Joback Method
cpg	437.50	J/molxK	687.12	Joback Method
cpg	450.30	J/molxK	722.34	Joback Method
cpg	462.32	J/molxK	757.56	Joback Method
cpg	473.55	J/molxK	792.78	Joback Method
dvisc	0.0021607	Paxs	321.10	Joback Method
dvisc	0.0010969	Paxs	364.50	Joback Method

dvisc	0.0006432	Paxs	407.89	Joback Method
dvisc	0.0004180	Paxs	451.29	Joback Method
dvisc	0.0002929	Paxs	494.68	Joback Method
dvisc	0.0002174	Paxs	538.08	Joback Method
dvisc	0.0001687	Paxs	581.47	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=U354637&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354637&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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