

# Propionic acid, 3-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C11H14O2/c1-3-9-6-5-7-10(8-9)13-11(12)4-2/h5-8H,3-4H2,1-2H3
<b>InchiKey:</b>	IHWMLAOSOIZYLB-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O2
<b>SMILES:</b>	CCC(=O)Oc1cccc(CC)c1
<b>Mol. weight [g/mol]:</b>	178.23

## Physical Properties

Property code	Value	Unit	Source
gf	-89.40	kJ/mol	Joback Method
hf	-290.11	kJ/mol	Joback Method
hfus	20.69	kJ/mol	Joback Method
hvap	52.17	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.564		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
rinpol	1359.00		NIST Webbook
tb	559.03	K	Joback Method
tc	769.35	K	Joback Method
tf	324.83	K	Joback Method
vc	0.568	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.15	J/molxK	559.03	Joback Method
cpg	409.50	J/molxK	734.30	Joback Method
cpg	398.29	J/molxK	699.24	Joback Method
cpg	386.36	J/molxK	664.19	Joback Method
cpg	373.70	J/molxK	629.14	Joback Method
cpg	360.31	J/molxK	594.08	Joback Method
cpg	420.01	J/molxK	769.35	Joback Method
dvisc	0.0001955	Paxs	559.03	Joback Method
dvisc	0.0002455	Paxs	520.00	Joback Method

dvisc	0.0003200	Paxs	480.96	Joback Method
dvisc	0.0004369	Paxs	441.93	Joback Method
dvisc	0.0006338	Paxs	402.90	Joback Method
dvisc	0.0009957	Paxs	363.86	Joback Method
dvisc	0.0017437	Paxs	324.83	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=U360698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360698&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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