

# 2-Ethylbutyric acid, 2-ethylphenyl ester

<b>Inchi:</b>	InChI=1S/C14H20O2/c1-4-11(5-2)14(15)16-13-10-8-7-9-12(13)6-3/h7-11H,4-6H2,1-3H3
<b>InchiKey:</b>	DCWBBPOIWJCPGN-UHFFFAOYSA-N
<b>Formula:</b>	C14H20O2
<b>SMILES:</b>	CCc1ccccc1OC(=O)C(CC)CC
<b>Mol. weight [g/mol]:</b>	220.31

## Physical Properties

Property code	Value	Unit	Source
gf	-66.58	kJ/mol	Joback Method
hf	-357.31	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	58.46	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.591		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	627.23	K	Joback Method
tc	832.03	K	Joback Method
tf	343.64	K	Joback Method
vc	0.730	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.28	J/molxK	627.23	Joback Method
cpg	510.76	J/molxK	661.36	Joback Method
cpg	526.32	J/molxK	695.50	Joback Method
cpg	540.99	J/molxK	729.63	Joback Method
cpg	554.78	J/molxK	763.76	Joback Method
cpg	567.73	J/molxK	797.90	Joback Method
cpg	579.84	J/molxK	832.03	Joback Method
dvisc	0.0019801	Paxs	343.64	Joback Method

dvisc	0.0009738	Paxs	390.90	Joback Method
dvisc	0.0005582	Paxs	438.17	Joback Method
dvisc	0.0003565	Paxs	485.44	Joback Method
dvisc	0.0002466	Paxs	532.70	Joback Method
dvisc	0.0001811	Paxs	579.97	Joback Method
dvisc	0.0001394	Paxs	627.23	Joback Method

## Sources

<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=U370260&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370260&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>

## 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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