

# Fumaric acid, 2-ethylbutyl pentyl ester

<b>Inchi:</b>	InChI=1S/C15H26O4/c1-4-7-8-11-18-14(16)9-10-15(17)19-12-13(5-2)6-3/h9-10,13H,4-8,
<b>InchiKey:</b>	GWQARORBJAUOTH-MDZDMXLPSA-N
<b>Formula:</b>	C15H26O4
<b>SMILES:</b>	CCCCCOC(=O)C=CC(=O)OCC(CC)CC
<b>Mol. weight [g/mol]:</b>	270.36

## Physical Properties

Property code	Value	Unit	Source
gf	-314.64	kJ/mol	Joback Method
hf	-730.59	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	66.87	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.255		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1592.35	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	698.90	K	Joback Method
tc	881.96	K	Joback Method
tf	383.05	K	Joback Method
vc	0.897	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.15	J/mol×K	698.90	Joback Method
cpg	671.00	J/mol×K	729.41	Joback Method
cpg	686.05	J/mol×K	759.92	Joback Method
cpg	700.31	J/mol×K	790.43	Joback Method
cpg	713.80	J/mol×K	820.94	Joback Method
cpg	726.53	J/mol×K	851.45	Joback Method
cpg	738.52	J/mol×K	881.96	Joback Method
dvisc	0.0015587	Paxs	383.05	Joback Method

dvisc	0.0007144	Paxs	435.69	Joback Method
dvisc	0.0003874	Paxs	488.33	Joback Method
dvisc	0.0002366	Paxs	540.98	Joback Method
dvisc	0.0001578	Paxs	593.62	Joback Method
dvisc	0.0001124	Paxs	646.26	Joback Method
dvisc	0.0000842	Paxs	698.90	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=U348295&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348295&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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