

# Fumaric acid, 3-ethylphenyl isoheptyl ester

<b>Inchi:</b>	InChI=1S/C18H24O4/c1-4-15-8-5-9-16(13-15)22-18(20)11-10-17(19)21-12-6-7-14(2)3/h5
<b>InchiKey:</b>	SZAGDLKJPXTXIU-ZHACJKMWSA-N
<b>Formula:</b>	C18H24O4
<b>SMILES:</b>	CCc1cccc(OC(=O)C=CC(=O)OCCCC(C)C)c1
<b>Mol. weight [g/mol]:</b>	304.38

## Physical Properties

Property code	Value	Unit	Source
gf	-186.60	kJ/mol	Joback Method
hf	-567.45	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	76.48	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.690		Crippen Method
mvol	251.300	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook
tb	799.20	K	Joback Method
tc	1006.70	K	Joback Method
tf	455.80	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.28	J/molxK	799.20	Joback Method
cpg	802.92	J/molxK	972.11	Joback Method
cpg	791.58	J/molxK	937.53	Joback Method
cpg	779.27	J/molxK	902.95	Joback Method
cpg	765.97	J/molxK	868.37	Joback Method
cpg	751.65	J/molxK	833.78	Joback Method
cpg	813.34	J/molxK	1006.70	Joback Method
dvisc	0.0000575	Paxs	799.20	Joback Method

dvisc	0.0000749	Paxs	741.97	Joback Method
dvisc	0.0001020	Paxs	684.73	Joback Method
dvisc	0.0001468	Paxs	627.50	Joback Method
dvisc	0.0002275	Paxs	570.27	Joback Method
dvisc	0.0003887	Paxs	513.03	Joback Method
dvisc	0.0007598	Paxs	455.80	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U348160&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348160&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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