

# Fumaric acid, 2-butyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C23H42O4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-20-26-22(24)18-19-23(25)2
<b>InchiKey:</b>	MXEXYKONXBTJMF-VHEBQXMUSA-N
<b>Formula:</b>	C23H42O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CC
<b>Mol. weight [g/mol]:</b>	382.58

## Physical Properties

Property code	Value	Unit	Source
gf	-247.28	kJ/mol	Joback Method
hf	-895.71	kJ/mol	Joback Method
hfus	57.58	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.519		Crippen Method
mvol	345.510	ml/mol	McGowan Method
pc	932.92	kPa	Joback Method
rinpol	2617.00		NIST Webbook
tb	881.94	K	Joback Method
tc	1079.77	K	Joback Method
tf	473.21	K	Joback Method
vc	1.345	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.31	J/molxK	881.94	Joback Method
cpg	1147.33	J/molxK	914.91	Joback Method
cpg	1165.14	J/molxK	947.88	Joback Method
cpg	1181.78	J/molxK	980.86	Joback Method
cpg	1197.28	J/molxK	1013.83	Joback Method
cpg	1211.70	J/molxK	1046.80	Joback Method
cpg	1225.06	J/molxK	1079.77	Joback Method
dvisc	0.0006444	Paxs	473.21	Joback Method
dvisc	0.0002732	Paxs	541.33	Joback Method

dvisc	0.0001403	Paxs	609.45	Joback Method
dvisc	0.0000824	Paxs	677.58	Joback Method
dvisc	0.0000533	Paxs	745.70	Joback Method
dvisc	0.0000371	Paxs	813.82	Joback Method
dvisc	0.0000273	Paxs	881.94	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=U348652&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348652&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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