

# Fumaric acid, eicosyl 3-oxobut-2-yl ester

<b>Inchi:</b>	InChI=1S/C28H50O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-32-27(30
<b>InchiKey:</b>	BWTNKSUSUHLXIP-GHVJWSGMSA-N
<b>Formula:</b>	C28H50O5
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	466.69

## Physical Properties

Property code	Value	Unit	Source
gf	-334.10	kJ/mol	Joback Method
hf	-1111.49	kJ/mol	Joback Method
hfus	72.13	kJ/mol	Joback Method
hvap	102.55	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.648		Crippen Method
mcvol	417.530	ml/mol	McGowan Method
pc	734.03	kPa	Joback Method
rinpol	3264.00		NIST Webbook
tb	1050.21	K	Joback Method
tc	1304.62	K	Joback Method
tf	579.49	K	Joback Method
vc	1.631	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1464.46	J/molxK	1050.21	Joback Method
cpg	1546.67	J/molxK	1262.22	Joback Method
cpg	1533.74	J/molxK	1219.82	Joback Method
cpg	1519.16	J/molxK	1177.42	Joback Method
cpg	1502.82	J/molxK	1135.01	Joback Method
cpg	1484.62	J/molxK	1092.61	Joback Method
cpg	1558.06	J/molxK	1304.62	Joback Method
dvisc	0.0000117	Paxs	1050.21	Joback Method
dvisc	0.0000158	Paxs	971.76	Joback Method

dvisc	0.0000226	Paxs	893.30	Joback Method
dvisc	0.0000345	Paxs	814.85	Joback Method
dvisc	0.0000578	Paxs	736.40	Joback Method
dvisc	0.0001095	Paxs	657.94	Joback Method
dvisc	0.0002466	Paxs	579.49	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=U348834&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348834&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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