

# Fumaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl pentadecyl ester

<b>Inchi:</b>	InChI=1S/C24H36F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-35-19(33)15-16-20(34)36
<b>InchiKey:</b>	VZFGREUICPMQJL-FOCLMDBBSA-N
<b>Formula:</b>	C24H36F8O4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
<b>Mol. weight [g/mol]:</b>	540.53

## Physical Properties

Property code	Value	Unit	Source
gf	-1788.82	kJ/mol	Joback Method
hf	-2511.48	kJ/mol	Joback Method
hfus	62.57	kJ/mol	Joback Method
hvap	76.48	kJ/mol	Joback Method
log10ws	-8.70		Crippen Method
logp	7.891		Crippen Method
mcvol	373.760	ml/mol	McGowan Method
pc	741.24	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	889.29	K	Joback Method
tc	1096.45	K	Joback Method
tf	496.46	K	Joback Method
vc	1.512	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.27	J/mol×K	889.29	Joback Method
cpg	1266.75	J/mol×K	923.82	Joback Method
cpg	1284.04	J/mol×K	958.34	Joback Method
cpg	1300.25	J/mol×K	992.87	Joback Method
cpg	1315.50	J/mol×K	1027.40	Joback Method
cpg	1329.91	J/mol×K	1061.93	Joback Method
cpg	1343.57	J/mol×K	1096.45	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=U348791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348791&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rinpola:</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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