

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

Inchi: InChI=1S/C15H18F8O4/c1-2-3-4-5-8-26-10(24)6-7-11(25)27-9-13(18,19)15(22,23)14(20)

InchiKey: ZNGQKDGFMRTACP-VOTSOKGWSA-N

Formula: C15H18F8O4

SMILES: CCCCCCOC(=O)C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 414.29

## Physical Properties

Property code	Value	Unit	Source
gf	-1864.60	kJ/mol	Joback Method
hf	-2325.72	kJ/mol	Joback Method
hfus	39.26	kJ/mol	Joback Method
hvap	56.44	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.380		Crippen Method
mvol	246.950	ml/mol	McGowan Method
pc	1267.35	kPa	Joback Method
rinpol	1674.00		NIST Webbook
rinpol	1674.00		NIST Webbook
tb	683.37	K	Joback Method
tc	845.85	K	Joback Method
tf	395.03	K	Joback Method
vc	1.008	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.64	J/mol×K	683.37	Joback Method
cpg	738.76	J/mol×K	710.45	Joback Method
cpg	751.11	J/mol×K	737.53	Joback Method
cpg	762.74	J/mol×K	764.61	Joback Method
cpg	773.67	J/mol×K	791.69	Joback Method
cpg	783.95	J/mol×K	818.77	Joback Method
cpg	793.62	J/mol×K	845.85	Joback Method

# Sources

<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=U348782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348782&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>

# 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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