

# Fumaric acid, pentafluorobenzyl 3-methylbut-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H15F5O4/c1-7(2)8(3)25-11(23)5-4-10(22)24-6-9-12(17)14(19)16(21)15(20)
<b>InchiKey:</b>	JNSRMZNTUSLMNI-SNAWJCMRSA-N
<b>Formula:</b>	C16H15F5O4
<b>SMILES:</b>	CC(C)C(C)OC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	366.28

## Physical Properties

Property code	Value	Unit	Source
gf	-1218.45	kJ/mol	Joback Method
hf	-1557.88	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	70.20	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.569		Crippen Method
mcvol	231.970	ml/mol	McGowan Method
pc	1522.31	kPa	Joback Method
rinpol	1850.00		NIST Webbook
rinpol	1850.00		NIST Webbook
tb	769.27	K	Joback Method
tc	956.44	K	Joback Method
tf	471.29	K	Joback Method
vc	0.929	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.56	J/molxK	769.27	Joback Method
cpg	671.75	J/molxK	800.46	Joback Method
cpg	683.18	J/molxK	831.66	Joback Method
cpg	693.85	J/molxK	862.85	Joback Method
cpg	703.78	J/molxK	894.05	Joback Method
cpg	712.95	J/molxK	925.24	Joback Method
cpg	721.39	J/molxK	956.44	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=U405876&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405876&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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