

# Diglycolic acid, pentafluorobenzyl pentyl ester

<b>Inchi:</b>	InChI=1S/C16H17F5O5/c1-2-3-4-5-25-10(22)7-24-8-11(23)26-6-9-12(17)14(19)16(21)15
<b>InchiKey:</b>	TYHBEPFLIRRVHS-UHFFFAOYSA-N
<b>Formula:</b>	C16H17F5O5
<b>SMILES:</b>	CCCCCOC(=O)COCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	384.30

## Physical Properties

Property code	Value	Unit	Source
gf	-1398.79	kJ/mol	Joback Method
hf	-1796.76	kJ/mol	Joback Method
hfus	51.45	kJ/mol	Joback Method
hvap	73.43	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.175		Crippen Method
mvol	242.140	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rmpol	2450.00		NIST Webbook
rmpol	2450.00		NIST Webbook
tb	788.41	K	Joback Method
tc	970.80	K	Joback Method
tf	528.60	K	Joback Method
vc	0.980	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.72	J/molxK	788.41	Joback Method
cpg	723.13	J/molxK	818.81	Joback Method
cpg	734.73	J/molxK	849.21	Joback Method
cpg	745.52	J/molxK	879.60	Joback Method
cpg	755.48	J/molxK	910.00	Joback Method
cpg	764.58	J/molxK	940.40	Joback Method
cpg	772.84	J/molxK	970.80	Joback Method

# Sources

<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>
<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=U382073&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U382073&amp;Units=SI</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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