

# Pimelic acid, isobutyl pentafluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C18H21F5O4/c1-10(2)8-26-12(24)6-4-3-5-7-13(25)27-9-11-14(19)16(21)18(23)
<b>InchiKey:</b>	NDQXTQIMMHLMJK-UHFFFAOYSA-N
<b>Formula:</b>	C18H21F5O4
<b>SMILES:</b>	CC(C)COC(=O)CCCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	396.35

## Physical Properties

Property code	Value	Unit	Source
gf	-1279.39	kJ/mol	Joback Method
hf	-1711.10	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	4.575		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	2115.00		NIST Webbook
rinpol	2115.00		NIST Webbook
tb	811.31	K	Joback Method
tc	996.92	K	Joback Method
tf	513.91	K	Joback Method
vc	1.067	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.29	J/molxK	811.31	Joback Method
cpg	809.86	J/molxK	842.25	Joback Method
cpg	822.54	J/molxK	873.18	Joback Method
cpg	834.32	J/molxK	904.12	Joback Method
cpg	845.21	J/molxK	935.05	Joback Method
cpg	855.21	J/molxK	965.99	Joback Method
cpg	864.31	J/molxK	996.92	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=U416626&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416626&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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