

# Diethylmalonic acid, isobutyl pentafluorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H19F5O4/c1-5-17(6-2,15(23)25-7-8(3)4)16(24)26-14-12(21)10(19)9(18)11
<b>InchiKey:</b>	FCRIDQLBLBOJJQ-UHFFFAOYSA-N
<b>Formula:</b>	C17H19F5O4
<b>SMILES:</b>	CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1c(F)c(F)c(F)c(F)c1F
<b>Mol. weight [g/mol]:</b>	382.32

## Physical Properties

Property code	Value	Unit	Source
gf	-1284.97	kJ/mol	Joback Method
hf	-1699.21	kJ/mol	Joback Method
hfus	41.92	kJ/mol	Joback Method
hvap	71.56	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.293		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1679.00		NIST Webbook
tb	785.20	K	Joback Method
tc	972.14	K	Joback Method
tf	505.06	K	Joback Method
vc	1.000	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.46	J/molxK	785.20	Joback Method
cpg	754.58	J/molxK	816.36	Joback Method
cpg	766.86	J/molxK	847.51	Joback Method
cpg	778.29	J/molxK	878.67	Joback Method
cpg	788.90	J/molxK	909.82	Joback Method
cpg	798.69	J/molxK	940.98	Joback Method
cpg	807.68	J/molxK	972.14	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=U370210&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370210&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>hvp:</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>rinp:</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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