

# Diethylmalonic acid, 3-fluorophenyl isobutyl ester

Inchi:	InChI=1S/C17H23FO4/c1-5-17(6-2,15(19)21-11-12(3)4)16(20)22-14-9-7-8-13(18)10-14/h
InchiKey:	BTPJXFROOBGCLD-UHFFFAOYSA-N
Formula:	C17H23FO4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]:	310.36

## Physical Properties

Property code	Value	Unit	Source
gf	-467.21	kJ/mol	Joback Method
hf	-868.89	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	72.19	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.737		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinsol	1820.00		NIST Webbook
tb	768.20	K	Joback Method
tc	972.60	K	Joback Method
tf	452.62	K	Joback Method
vc	0.928	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.41	J/molxK	768.20	Joback Method
cpg	729.75	J/molxK	802.27	Joback Method
cpg	744.04	J/molxK	836.33	Joback Method
cpg	757.30	J/molxK	870.40	Joback Method
cpg	769.56	J/molxK	904.46	Joback Method
cpg	780.86	J/molxK	938.53	Joback Method
cpg	791.23	J/molxK	972.60	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U370197&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370197&amp;Units=SI</a>
<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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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