

# Diethylmalonic acid, ethyl 3,4,5-trifluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C16H19F3O4/c1-4-16(5-2,14(20)22-6-3)15(21)23-9-10-7-11(17)13(19)12(18)8
<b>InchiKey:</b>	QXLMXISDEWZNRB-UHFFFAOYSA-N
<b>Formula:</b>	C16H19F3O4
<b>SMILES:</b>	CCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	332.31

## Physical Properties

Property code	Value	Unit	Source
gf	-882.07	kJ/mol	Joback Method
hf	-1258.13	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.517		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
tb	754.26	K	Joback Method
tc	946.60	K	Joback Method
tf	482.57	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.04	J/mol×K	754.26	Joback Method
cpg	685.63	J/mol×K	786.32	Joback Method
cpg	698.35	J/mol×K	818.37	Joback Method
cpg	710.22	J/mol×K	850.43	Joback Method
cpg	721.25	J/mol×K	882.48	Joback Method
cpg	731.47	J/mol×K	914.54	Joback Method
cpg	740.89	J/mol×K	946.60	Joback Method

# Sources

<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=U369272&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369272&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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