

# Diethylmalonic acid, pentafluorobenzyl tridecyl ester

Inchi:	InChI=1S/C27H39F5O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-35-25(33)27(5-2,6-3)26(34)
InchiKey:	DPADUJMSLSQPAS-UHFFFAOYSA-N
Formula:	C27H39F5O4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	522.59

## Physical Properties

Property code	Value	Unit	Source
gf	-1198.33	kJ/mol	Joback Method
hf	-1900.33	kJ/mol	Joback Method
hfus	71.34	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-9.86		Crippen Method
logp	8.086		Crippen Method
mcvol	391.260	ml/mol	McGowan Method
pc	743.26	kPa	Joback Method
rinpol	2645.00		NIST Webbook
rinpol	2645.00		NIST Webbook
tb	1014.44	K	Joback Method
tc	1257.63	K	Joback Method
tf	632.76	K	Joback Method
vc	1.567	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1337.14	J/molxK	1014.44	Joback Method
cpg	1354.73	J/molxK	1054.97	Joback Method
cpg	1370.51	J/molxK	1095.50	Joback Method
cpg	1384.53	J/molxK	1136.04	Joback Method
cpg	1396.87	J/molxK	1176.57	Joback Method
cpg	1407.61	J/molxK	1217.10	Joback Method
cpg	1416.81	J/molxK	1257.63	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=U369999&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369999&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>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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