

# Diethylmalonic acid, dodecyl 2-fluorophenyl ester

Inchi:	InChI=1S/C25H39FO4/c1-4-7-8-9-10-11-12-13-14-17-20-29-23(27)25(5-2,6-3)24(28)30-2
InchiKey:	OXTYZJISTBRADX-UHFFFAOYSA-N
Formula:	C25H39FO4
SMILES:	CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F
Mol. weight [g/mol]:	422.57

## Physical Properties

Property code	Value	Unit	Source
gf	-397.41	kJ/mol	Joback Method
hf	-1028.73	kJ/mol	Joback Method
hfus	55.40	kJ/mol	Joback Method
hvap	90.38	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.002		Crippen Method
mcvol	356.000	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	2682.00		NIST Webbook
rinpol	2682.00		NIST Webbook
tb	951.68	K	Joback Method
tc	1165.17	K	Joback Method
tf	557.78	K	Joback Method
vc	1.383	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.25	J/molxK	951.68	Joback Method
cpg	1205.33	J/molxK	987.26	Joback Method
cpg	1221.07	J/molxK	1022.84	Joback Method
cpg	1235.53	J/molxK	1058.42	Joback Method
cpg	1248.79	J/molxK	1094.01	Joback Method
cpg	1260.90	J/molxK	1129.59	Joback Method
cpg	1271.93	J/molxK	1165.17	Joback Method

# Sources

<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=U370136&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370136&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>

# 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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