

# Phthalic acid, decyl 2,5-difluorobenzyl ester

<b>Inchi:</b>	InChI=1S/C25H30F2O4/c1-2-3-4-5-6-7-8-11-16-30-24(28)21-12-9-10-13-22(21)25(29)31
<b>InchiKey:</b>	UFOAIKLYUOYMBH-UHFFFAOYSA-N
<b>Formula:</b>	C25H30F2O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
<b>Mol. weight [g/mol]:</b>	432.50

## Physical Properties

Property code	Value	Unit	Source
gf	-501.91	kJ/mol	Joback Method
hf	-1002.50	kJ/mol	Joback Method
hfus	59.15	kJ/mol	Joback Method
hvap	94.46	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	6.619		Crippen Method
mvol	334.010	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2838.00		NIST Webbook
rinpol	2838.00		NIST Webbook
tb	990.82	K	Joback Method
tc	1213.56	K	Joback Method
tf	607.41	K	Joback Method
vc	1.304	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.57	J/mol×K	990.82	Joback Method
cpg	1102.32	J/mol×K	1027.94	Joback Method
cpg	1114.64	J/mol×K	1065.07	Joback Method
cpg	1125.57	J/mol×K	1102.19	Joback Method
cpg	1135.15	J/mol×K	1139.31	Joback Method
cpg	1143.44	J/mol×K	1176.44	Joback Method
cpg	1150.47	J/mol×K	1213.56	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377807&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377807&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.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>
<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>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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