

# Phthalic acid, tridecyl 2,4,5-trifluorobenzyl ester

Inchi:	InChI=1S/C28H35F3O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-34-27(32)22-15-12-13-16-23(22)
InchiKey:	GMMQMBSUEYATKJ-UHFFFAOYSA-N
Formula:	C28H35F3O4
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]:	492.57

## Physical Properties

Property code	Value	Unit	Source
gf	-681.09	kJ/mol	Joback Method
hf	-1272.00	kJ/mol	Joback Method
hfus	69.62	kJ/mol	Joback Method
hvap	100.98	kJ/mol	Joback Method
log10ws	-10.08		Crippen Method
logp	7.929		Crippen Method
mvol	378.050	ml/mol	McGowan Method
pc	892.67	kPa	Joback Method
rinpol	3370.00		NIST Webbook
rinpol	3370.00		NIST Webbook
tb	1063.71	K	Joback Method
tc	1307.16	K	Joback Method
tf	654.33	K	Joback Method
vc	1.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.68	J/molxK	1063.71	Joback Method
cpg	1290.68	J/molxK	1104.28	Joback Method
cpg	1302.89	J/molxK	1144.86	Joback Method
cpg	1313.37	J/molxK	1185.43	Joback Method
cpg	1322.18	J/molxK	1226.01	Joback Method
cpg	1329.39	J/molxK	1266.58	Joback Method
cpg	1335.08	J/molxK	1307.16	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=U415503&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415503&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>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>rlnol:</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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