

# Phthalic acid, dodecyl 4-trifluoromethoxybenzyl ester

Inchi:	InChI=1S/C28H35F3O5/c1-2-3-4-5-6-7-8-9-10-13-20-34-26(32)24-14-11-12-15-25(24)27
InchiKey:	CAWNGDUOKPWJEA-UHFFFAOYSA-N
Formula:	C28H35F3O5
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	508.57

## Physical Properties

Property code	Value	Unit	Source
gf	-763.99	kJ/mol	Joback Method
hf	-1390.03	kJ/mol	Joback Method
hfus	64.17	kJ/mol	Joback Method
hvap	100.77	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	8.020		Crippen Method
mvol	383.920	ml/mol	McGowan Method
pc	909.98	kPa	Joback Method
rinpol	3084.00		NIST Webbook
rinpol	3084.00		NIST Webbook
tb	1072.94	K	Joback Method
tc	1317.23	K	Joback Method
tf	653.94	K	Joback Method
vc	1.496	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.59	J/molxK	1072.94	Joback Method
cpg	1319.03	J/molxK	1113.66	Joback Method
cpg	1330.78	J/molxK	1154.37	Joback Method
cpg	1340.92	J/molxK	1195.09	Joback Method
cpg	1349.56	J/molxK	1235.80	Joback Method
cpg	1356.77	J/molxK	1276.52	Joback Method
cpg	1362.66	J/molxK	1317.23	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=U377694&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377694&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>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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