

# Phthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl undecyl ester

<b>Inchi:</b>	InChI=1S/C23H29F7O4/c1-2-3-4-5-6-7-8-9-12-15-33-19(31)17-13-10-11-14-18(17)20(32)
<b>InchiKey:</b>	RSIZNCDJZGTHRS-UHFFFAOYSA-N
<b>Formula:</b>	C23H29F7O4
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1cccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	502.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1577.43	kJ/mol	Joback Method
hf	-2181.61	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.364		Crippen Method
mvol	338.440	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	895.08	K	Joback Method
tc	1095.92	K	Joback Method
tf	543.62	K	Joback Method
vc	1.357	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.26	J/molxK	895.08	Joback Method
cpg	1124.41	J/molxK	928.55	Joback Method
cpg	1138.49	J/molxK	962.03	Joback Method
cpg	1151.60	J/molxK	995.50	Joback Method
cpg	1163.82	J/molxK	1028.97	Joback Method
cpg	1175.23	J/molxK	1062.45	Joback Method
cpg	1185.93	J/molxK	1095.92	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=U415549&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415549&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>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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