

# Terephthalic acid, heptadecyl 2,2,3,3,4,4,4-heptafluorobutyl ester

**Inchi:** InChI=1S/C29H41F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-39-25(37)23-17-19  
**InchiKey:** SPHRMZSFFHZQPF-UHFFFAOYSA-N  
**Formula:** C29H41F7O4  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)F)cc1  
**Mol. weight [g/mol]:** 586.62

## Physical Properties

Property code	Value	Unit	Source
gf	-1526.91	kJ/mol	Joback Method
hf	-2305.45	kJ/mol	Joback Method
hfus	69.41	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.704		Crippen Method
mvol	422.980	ml/mol	McGowan Method
pc	673.95	kPa	Joback Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	1032.36	K	Joback Method
tc	1287.24	K	Joback Method
tf	611.24	K	Joback Method
vc	1.692	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1478.69	J/molxK	1032.36	Joback Method
cpg	1498.05	J/molxK	1074.84	Joback Method
cpg	1515.97	J/molxK	1117.32	Joback Method
cpg	1532.67	J/molxK	1159.80	Joback Method
cpg	1548.34	J/molxK	1202.28	Joback Method
cpg	1563.20	J/molxK	1244.76	Joback Method
cpg	1577.47	J/molxK	1287.24	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U415949&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415949&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.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>

# 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

Latest version available from:

<https://www.chemeo.com/cid/121-392-2/Terephthalic-acid-heptadecyl-2-2-3-3-4-4-4-heptafluorobutyl-ester.pdf>

Generated by Cheméo on 2024-05-02 20:56:53.765312888 +0000 UTC m=+16972662.685890200.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.