

# Terephthalic acid, tetradecyl 2,2,2-trifluoroethyl ester

Inchi:	InChI=1S/C24H35F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-30-22(28)20-14-16-21(17-15
InchiKey:	NWRPNPSCJVYXQY-UHFFFAOYSA-N
Formula:	C24H35F3O4
SMILES:	CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
Mol. weight [g/mol]:	444.53

## Physical Properties

Property code	Value	Unit	Source
gf	-795.45	kJ/mol	Joback Method
hf	-1400.31	kJ/mol	Joback Method
hfus	58.97	kJ/mol	Joback Method
hvap	86.52	kJ/mol	Joback Method
log10ws	-8.48		Crippen Method
logp	7.264		Crippen Method
mvol	345.450	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2946.00		NIST Webbook
rinpol	2946.00		NIST Webbook
tb	927.34	K	Joback Method
tc	1135.40	K	Joback Method
tf	547.69	K	Joback Method
vc	1.363	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.63	J/mol×K	927.34	Joback Method
cpg	1157.09	J/mol×K	962.02	Joback Method
cpg	1172.28	J/mol×K	996.69	Joback Method
cpg	1186.27	J/mol×K	1031.37	Joback Method
cpg	1199.10	J/mol×K	1066.04	Joback Method
cpg	1210.85	J/mol×K	1100.72	Joback Method
cpg	1221.57	J/mol×K	1135.40	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U383049&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U383049&amp;Units=SI</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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