

# Terephthalic acid, heptyl 3-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C20H30O4/c1-4-5-6-7-8-14-23-19(21)17-9-11-18(12-10-17)20(22)24-15-13-16
<b>InchiKey:</b>	NKOTWPVEPQCIMK-UHFFFAOYSA-N
<b>Formula:</b>	C20H30O4
<b>SMILES:</b>	CCCCCCCOC(=O)c1ccc(C(=O)OCCC(C)C)cc1
<b>Mol. weight [g/mol]:</b>	334.45

## Physical Properties

Property code	Value	Unit	Source
gf	-249.98	kJ/mol	Joback Method
hf	-725.95	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	80.98	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.017		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	840.80	K	Joback Method
tc	1042.55	K	Joback Method
tf	483.42	K	Joback Method
vc	1.089	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.24	J/molxK	840.80	Joback Method
cpg	948.18	J/molxK	1008.93	Joback Method
cpg	936.41	J/molxK	975.30	Joback Method
cpg	923.56	J/molxK	941.68	Joback Method
cpg	909.59	J/molxK	908.05	Joback Method
cpg	894.49	J/molxK	874.43	Joback Method
cpg	958.87	J/molxK	1042.55	Joback Method
dvisc	0.0000502	Paxs	840.80	Joback Method

dvisc	0.0000656	Paxs	781.24	Joback Method
dvisc	0.0000897	Paxs	721.67	Joback Method
dvisc	0.0001295	Paxs	662.11	Joback Method
dvisc	0.0002012	Paxs	602.55	Joback Method
dvisc	0.0003442	Paxs	542.98	Joback Method
dvisc	0.0006723	Paxs	483.42	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=U356139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356139&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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