

# Terephthalic acid, butyl 2-phenoxyethyl ester

<b>Inchi:</b>	InChI=1S/C20H22O5/c1-2-3-13-24-19(21)16-9-11-17(12-10-16)20(22)25-15-14-23-18-7-
<b>InchiKey:</b>	ANRUEXZRMXQCKQ-UHFFFAOYSA-N
<b>Formula:</b>	C20H22O5
<b>SMILES:</b>	CCCCOC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1
<b>Mol. weight [g/mol]:</b>	342.39

## Physical Properties

Property code	Value	Unit	Source
gf	-240.13	kJ/mol	Joback Method
hf	-616.36	kJ/mol	Joback Method
hfus	42.01	kJ/mol	Joback Method
hvap	86.05	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.879		Crippen Method
mvol	265.890	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	2842.00		NIST Webbook
tb	890.34	K	Joback Method
tc	1113.35	K	Joback Method
tf	547.07	K	Joback Method
vc	1.006	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.72	J/molxK	890.34	Joback Method
cpg	862.71	J/molxK	1076.18	Joback Method
cpg	854.56	J/molxK	1039.01	Joback Method
cpg	845.10	J/molxK	1001.84	Joback Method
cpg	834.32	J/molxK	964.68	Joback Method
cpg	822.20	J/molxK	927.51	Joback Method
cpg	869.60	J/molxK	1113.35	Joback Method
dvisc	0.0000421	Paxs	890.34	Joback Method
dvisc	0.0000534	Paxs	833.13	Joback Method

dvisc	0.0000701	Paxs	775.92	Joback Method
dvisc	0.0000960	Paxs	718.70	Joback Method
dvisc	0.0001388	Paxs	661.49	Joback Method
dvisc	0.0002154	Paxs	604.28	Joback Method
dvisc	0.0003662	Paxs	547.07	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U416043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U416043&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>

## Legend

<b>cpg:</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>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>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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