

# N-butyl-o-benzoyl benzoate

<b>Inchi:</b>	InChI=1S/C18H18O3/c1-2-3-13-21-18(20)16-12-8-7-11-15(16)17(19)14-9-5-4-6-10-14/h
<b>InchiKey:</b>	VMHKPGQWBDCSM-UHFFFAOYSA-N
<b>Formula:</b>	C18H18O3
<b>SMILES:</b>	CCCCOC(=O)c1ccccc1C(=O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	282.33
<b>CAS:</b>	571-98-2

## Physical Properties

Property code	Value	Unit	Source
gf	-46.97	kJ/mol	Joback Method
hf	-310.64	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.874		Crippen Method
mcvol	225.970	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	799.74	K	Joback Method
tc	1030.70	K	Joback Method
tf	480.07	K	Joback Method
vc	0.858	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.46	J/molxK	799.74	Joback Method
cpg	655.99	J/molxK	838.23	Joback Method
cpg	669.31	J/molxK	876.73	Joback Method
cpg	681.46	J/molxK	915.22	Joback Method
cpg	692.51	J/molxK	953.71	Joback Method
cpg	702.51	J/molxK	992.20	Joback Method
cpg	711.51	J/molxK	1030.70	Joback Method
dvisc	0.0008645	Paxs	480.07	Joback Method
dvisc	0.0004996	Paxs	533.35	Joback Method

dvisc	0.0003189	Paxs	586.63	Joback Method
dvisc	0.0002194	Paxs	639.90	Joback Method
dvisc	0.0001599	Paxs	693.18	Joback Method
dvisc	0.0001219	Paxs	746.46	Joback Method
dvisc	0.0000963	Paxs	799.74	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C571982&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C571982&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>
<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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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