

# Benzoylcarboxyperoxide phenyl ester

<b>Inchi:</b>	InChI=1S/C14H10O5/c15-13(11-7-3-1-4-8-11)18-19-14(16)17-12-9-5-2-6-10-12/h1-10H
<b>InchiKey:</b>	WFSLLYWSMDDIAX-UHFFFAOYSA-N
<b>Formula:</b>	C14H10O5
<b>SMILES:</b>	O=C(OOC(=O)c1ccccc1)Oc1ccccc1
<b>Mol. weight [g/mol]:</b>	258.23
<b>CAS:</b>	962-16-3

## Physical Properties

Property code	Value	Unit	Source
chs	-6453.40 ± 8.40	kJ/mol	NIST Webbook
gf	-281.02	kJ/mol	Joback Method
hf	-393.00 ± 10.00	kJ/mol	NIST Webbook
hfs	-484.90 ± 8.40	kJ/mol	NIST Webbook
hfus	26.86	kJ/mol	Joback Method
hvap	72.03	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	2.974		Crippen Method
mcvol	181.350	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	748.08	K	Joback Method
tc	988.82	K	Joback Method
tf	466.93	K	Joback Method
vc	0.669	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.07	J/molxK	748.08	Joback Method
cpg	491.61	J/molxK	788.20	Joback Method
cpg	502.94	J/molxK	828.33	Joback Method
cpg	513.09	J/molxK	868.45	Joback Method
cpg	522.05	J/molxK	908.58	Joback Method
cpg	529.83	J/molxK	948.70	Joback Method
cpg	536.45	J/molxK	988.82	Joback Method

dvisc	0.0007231	Paxs	466.93	Joback Method
dvisc	0.0004390	Paxs	513.79	Joback Method
dvisc	0.0002898	Paxs	560.65	Joback Method
dvisc	0.0002039	Paxs	607.50	Joback Method
dvisc	0.0001509	Paxs	654.36	Joback Method
dvisc	0.0001163	Paxs	701.22	Joback Method
dvisc	0.0000925	Paxs	748.08	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=C962163&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C962163&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>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase 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>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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