

# «alpha»-Phenylglutaric anhydride

<b>Other names:</b>	2H-Pyran-2,6(3H)-dione, dihydro-3-phenyl-2-phenylglutaric anhydride
<b>Inchi:</b>	InChI=1S/C11H10O3/c12-10-7-6-9(11(13)14-10)8-4-2-1-3-5-8/h1-5,9H,6-7H2
<b>InchiKey:</b>	NVPRNSAYSSEIGR-UHFFFAOYSA-N
<b>Formula:</b>	C11H10O3
<b>SMILES:</b>	O=C1CCC(c2ccccc2)C(=O)O1
<b>Mol. weight [g/mol]:</b>	190.20
<b>CAS:</b>	2959-96-8

## Physical Properties

Property code	Value	Unit	Source
gf	-152.70	kJ/mol	Joback Method
hf	-386.92	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.634		Crippen Method
mvol	140.240	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	659.90	K	Joback Method
tc	930.80	K	Joback Method
tf	410.54	K	Joback Method
vc	0.511	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.59	J/molxK	659.90	Joback Method
cpg	394.12	J/molxK	705.05	Joback Method
cpg	410.21	J/molxK	750.20	Joback Method
cpg	424.82	J/molxK	795.35	Joback Method
cpg	437.89	J/molxK	840.50	Joback Method
cpg	449.39	J/molxK	885.65	Joback Method
cpg	459.26	J/molxK	930.80	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	1.70	NIST Webbook
tbrp	497.20	K	1.70	NIST Webbook

## 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=C2959968&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2959968&amp;Units=SI</a>
<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.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>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>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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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