

# Glutaric acid, but-3-yn-2-yl 3-phenoxybenzyl ester

<b>Inchi:</b>	InChI=1S/C22H22O5/c1-3-17(2)26-22(24)14-8-13-21(23)25-16-18-9-7-12-20(15-18)27-1
<b>InchiKey:</b>	BDDZTMKACAOCIR-UHFFFAOYSA-N
<b>Formula:</b>	C22H22O5
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1</chem>
<b>Mol. weight [g/mol]:</b>	366.41

## Physical Properties

Property code	Value	Unit	Source
gf	-2.66	kJ/mol	Joback Method
hf	-371.02	kJ/mol	Joback Method
hfus	46.64	kJ/mol	Joback Method
hvap	89.97	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.257		Crippen Method
mvol	285.470	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	925.78	K	Joback Method
tc	1156.84	K	Joback Method
tf	601.58	K	Joback Method
vc	1.073	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.89	J/mol×K	925.78	Joback Method
cpg	879.86	J/mol×K	964.29	Joback Method
cpg	891.43	J/mol×K	1002.80	Joback Method
cpg	901.63	J/mol×K	1041.31	Joback Method
cpg	910.51	J/mol×K	1079.82	Joback Method
cpg	918.10	J/mol×K	1118.33	Joback Method
cpg	924.44	J/mol×K	1156.84	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392122&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>hvp:</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>rinp:</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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