

# Morpholine-3-carboxylic acid, 2-phenyl, methyl ester, trans

Inchi:	InChI=1S/C12H15NO3/c1-15-12(14)10-11(16-8-7-13-10)9-5-3-2-4-6-9/h2-6,10-11,13H,7
InchiKey:	HZWHDMCEMDPHNT-MNOVXSKESA-N
Formula:	C12H15NO3
SMILES:	COC(=O)C1NCCOC1c1ccccc1
Mol. weight [g/mol]:	221.25

## Physical Properties

Property code	Value	Unit	Source
gf	-53.02	kJ/mol	Joback Method
hf	-359.49	kJ/mol	Joback Method
hfus	34.14	kJ/mol	Joback Method
hvap	65.13	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	0.889		Crippen Method
mvol	168.610	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1736.00		NIST Webbook
tb	667.31	K	Joback Method
tc	911.54	K	Joback Method
tf	458.32	K	Joback Method
vc	0.614	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.50	J/molxK	667.31	Joback Method
cpg	481.31	J/molxK	708.02	Joback Method
cpg	497.75	J/molxK	748.72	Joback Method
cpg	512.85	J/molxK	789.43	Joback Method
cpg	526.60	J/molxK	830.13	Joback Method
cpg	539.04	J/molxK	870.84	Joback Method
cpg	550.17	J/molxK	911.54	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=R331810&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331810&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>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>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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