

# 2-(4-cyclohexylmethoxy-phenyl)-propionic acid, methyl ester

Inchi:	InChI=1S/C17H18O3/c1-13(17(18)19-2)15-8-10-16(11-9-15)20-12-14-6-4-3-5-7-14/h3-11
InchiKey:	NYJKRTRWIXNPDP-UHFFFAOYSA-N
Formula:	C17H18O3
SMILES:	COC(=O)C(C)c1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	270.32

## Physical Properties

Property code	Value	Unit	Source
gf	-33.91	kJ/mol	Joback Method
hf	-314.92	kJ/mol	Joback Method
hfus	27.93	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.542		Crippen Method
mcvol	216.180	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
rinpol	2078.50		NIST Webbook
rinpol	2078.50		NIST Webbook
tb	744.97	K	Joback Method
tc	975.62	K	Joback Method
tf	426.10	K	Joback Method
vc	0.807	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.97	J/molxK	744.97	Joback Method
cpg	666.96	J/molxK	937.18	Joback Method
cpg	655.76	J/molxK	898.74	Joback Method
cpg	643.39	J/molxK	860.30	Joback Method
cpg	629.83	J/molxK	821.85	Joback Method
cpg	615.03	J/molxK	783.41	Joback Method
cpg	677.03	J/molxK	975.62	Joback Method
dvisc	0.0000778	Paxs	744.97	Joback Method

dvisc	0.0001002	Paxs	691.83	Joback Method
dvisc	0.0001347	Paxs	638.68	Joback Method
dvisc	0.0001909	Paxs	585.54	Joback Method
dvisc	0.0002901	Paxs	532.39	Joback Method
dvisc	0.0004838	Paxs	479.25	Joback Method
dvisc	0.0009165	Paxs	426.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R157850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R157850&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>
<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>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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