

# 2-Methylvaleric acid, cyclohexylmethyl ester

Inchi:	InChI=1S/C13H24O2/c1-3-7-11(2)13(14)15-10-12-8-5-4-6-9-12/h11-12H,3-10H2,1-2H3
InchiKey:	PGJSABZOWJTODI-UHFFFAOYSA-N
Formula:	C13H24O2
SMILES:	CCCC(C)C(=O)OCC1CCCCC1
Mol. weight [g/mol]:	212.33

## Physical Properties

Property code	Value	Unit	Source
gf	-153.33	kJ/mol	Joback Method
hf	-507.41	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.546		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1478.00		NIST Webbook
tb	592.24	K	Joback Method
tc	792.82	K	Joback Method
tf	300.81	K	Joback Method
vc	0.715	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.82	J/molxK	592.24	Joback Method
cpg	596.36	J/molxK	759.39	Joback Method
cpg	580.48	J/molxK	725.96	Joback Method
cpg	563.61	J/molxK	692.53	Joback Method
cpg	545.72	J/molxK	659.10	Joback Method
cpg	526.80	J/molxK	625.67	Joback Method
cpg	611.27	J/molxK	792.82	Joback Method
dvisc	0.0001699	Paxs	592.24	Joback Method
dvisc	0.0002320	Paxs	543.67	Joback Method

dvisc	0.0003368	Paxs	495.10	Joback Method
dvisc	0.0005301	Paxs	446.52	Joback Method
dvisc	0.0009321	Paxs	397.95	Joback Method
dvisc	0.0019175	Paxs	349.38	Joback Method
dvisc	0.0049796	Paxs	300.81	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U357760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357760&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>

## 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>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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