

# Heptanoic acid, phenylmethyl ester

<b>Other names:</b>	Benzyl n-heptanoate Benzyl heptanoate
<b>Inchi:</b>	InChI=1S/C14H20O2/c1-2-3-4-8-11-14(15)16-12-13-9-6-5-7-10-13/h5-7,9-10H,2-4,8,11-14
<b>InchiKey:</b>	UEDDAJQIHUEZCJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H20O2
<b>SMILES:</b>	CCCCCCC(=O)OCc1ccccc1
<b>Mol. weight [g/mol]:</b>	220.31
<b>CAS:</b>	5454-21-7

## Physical Properties

Property code	Value	Unit	Source
gf	-54.51	kJ/mol	Joback Method
hf	-340.56	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.700		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
ripol	2158.00		NIST Webbook
ripol	2158.00		NIST Webbook
tb	622.69	K	Joback Method
tc	822.76	K	Joback Method
tf	346.12	K	Joback Method
vc	0.736	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.13	J/molxK	622.69	Joback Method

cpg	510.47	J/molxK	656.04	Joback Method
cpg	525.89	J/molxK	689.38	Joback Method
cpg	540.43	J/molxK	722.73	Joback Method
cpg	554.11	J/molxK	756.07	Joback Method
cpg	566.96	J/molxK	789.42	Joback Method
cpg	579.01	J/molxK	822.76	Joback Method
dvisc	0.0020543	Paxs	346.12	Joback Method
dvisc	0.0010310	Paxs	392.21	Joback Method
dvisc	0.0005982	Paxs	438.31	Joback Method
dvisc	0.0003849	Paxs	484.40	Joback Method
dvisc	0.0002674	Paxs	530.50	Joback Method
dvisc	0.0001969	Paxs	576.60	Joback Method
dvisc	0.0001517	Paxs	622.69	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5454217&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5454217&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>

## 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>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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