

# 6-(benzo[d][1,3]dioxol-5-yl)hex-3-en-2-one

<b>Inchi:</b>	InChI=1S/C13H14O3/c1-10(14)4-2-3-5-11-6-7-12-13(8-11)16-9-15-12/h2,4,6-8H,3,5,9H2
<b>InchiKey:</b>	WBTCWBZQKZZDOV-DUXPYHPUSA-N
<b>Formula:</b>	C13H14O3
<b>SMILES:</b>	CC(=O)C=CCCc1ccc2c(c1)OCO2
<b>Mol. weight [g/mol]:</b>	218.25
<b>CAS:</b>	75787-97-2

## Physical Properties

Property code	Value	Unit	Source
gf	-0.75	kJ/mol	Joback Method
hf	-264.28	kJ/mol	Joback Method
hfus	37.51	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.493		Crippen Method
mcvol	168.420	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	656.82	K	Joback Method
tc	882.74	K	Joback Method
tf	407.90	K	Joback Method
vc	0.641	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.84	J/molxK	656.82	Joback Method
cpg	498.64	J/molxK	845.09	Joback Method
cpg	488.24	J/molxK	807.43	Joback Method
cpg	477.15	J/molxK	769.78	Joback Method
cpg	465.27	J/molxK	732.13	Joback Method
cpg	452.53	J/molxK	694.47	Joback Method
cpg	508.44	J/molxK	882.74	Joback Method

dvisc	0.0003392	Paxs	656.82	Joback Method
dvisc	0.0004111	Paxs	615.33	Joback Method
dvisc	0.0005123	Paxs	573.85	Joback Method
dvisc	0.0006607	Paxs	532.36	Joback Method
dvisc	0.0008895	Paxs	490.87	Joback Method
dvisc	0.0012653	Paxs	449.39	Joback Method
dvisc	0.0019334	Paxs	407.90	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C75787972&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C75787972&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>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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