

# Fenchyl acetate

<b>Other names:</b>	Bicyclo[2.2.1]heptan-2-ol, 1,3,3-trimethyl-, acetate 1,3,3-Trimethyl-2-norbornanyl acetate 2-Norbornanol, 1,3,3-trimethyl-, acetate 1,3,3-Trimethylbicyclo[2.2.1]hept-2-yl acetate NSC 404295 Fenchyl acetate (Isomer) 3,3-dimethyl-8,9-dinorbornan-2-yl acetate
<b>Inchi:</b>	InChI=1S/C12H20O2/c1-8(13)14-10-11(2,3)9-5-6-12(10,4)7-9/h9-10H,5-7H2,1-4H3
<b>InchiKey:</b>	JUWUWIGZUVEFQB-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	CC(=O)OC1C2(C)CCC(C2)C1(C)C
<b>Mol. weight [g/mol]:</b>	196.29
<b>CAS:</b>	13851-11-1

## Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-406.57	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1209.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1211.00		NIST Webbook
rinpol	1225.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1199.00		NIST Webbook

rinpol	1198.00	NIST Webbook
rinpol	1232.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1204.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1219.00	NIST Webbook
rinpol	1240.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1212.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1232.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1205.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1214.00	NIST Webbook
rinpol	1207.00	NIST Webbook
rinpol	1217.00	NIST Webbook
rinpol	1208.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1208.00	NIST Webbook
rinpol	1206.00	NIST Webbook
rinpol	1208.00	NIST Webbook
rinpol	1222.60	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1233.00	NIST Webbook
rinpol	1210.00	NIST Webbook
rinpol	1220.00	NIST Webbook
ripol	1481.00	NIST Webbook
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ripol	1460.00	NIST Webbook
ripol	1473.00	NIST Webbook
ripol	1466.00	NIST Webbook
ripol	1473.00	NIST Webbook
ripol	1426.00	NIST Webbook
ripol	1458.00	NIST Webbook
ripol	1482.00	NIST Webbook

ripol	1443.00		NIST Webbook
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ripol	1468.00		NIST Webbook
ripol	1466.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1464.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1464.00		NIST Webbook
tb	559.14	K	Joback Method
tc	774.82	K	Joback Method
tf	368.84	K	Joback Method
vc	0.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.90	J/mol×K	559.14	Joback Method
cpg	456.54	J/mol×K	595.09	Joback Method
cpg	474.00	J/mol×K	631.03	Joback Method
cpg	490.47	J/mol×K	666.98	Joback Method
cpg	506.18	J/mol×K	702.93	Joback Method
cpg	521.34	J/mol×K	738.88	Joback Method
cpg	536.18	J/mol×K	774.82	Joback Method

## Sources

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13851111&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	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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