

# Butanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E)-

Other names:

Geranyl 2-methylbutyrate  
Geranyl 2-methylbutanoate  
(E)-Anyl 2-methylbutyrate  
(E)-3,7-dimethylocta-2,6-dienyl 2-methylbutyrate

Inchi:

InChI=1S/C15H26O2/c1-6-14(5)15(16)17-11-10-13(4)9-7-8-12(2)3/h8,10,14H,6-7,9,11H2

InchiKey:

PEQMAZJTEUEQJP-JLHYYAGUSA-N

Formula:

C15H26O2

SMILES:

CCC(C)C(=O)OCC=C(C)CCC=C(C)C

Mol. weight [g/mol]:

238.37

CAS:

68705-63-5

## Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.268		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1596.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1579.00		NIST Webbook
rinpol	1584.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1904.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1904.00		NIST Webbook

ripol	1886.00		NIST Webbook
ripol	1880.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method
cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C68705635&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)

**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>

## 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</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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