2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, acetate, (E,E)-

Other names: all-trans-Farnesyl acetate
trans, trans-Farnesyl acetate
2-trans-6-trans-Farnesyl acetate
(2E,6E)-Farnesyl acetate
trans,trans-Farnesol acetate
[(E,E)-3,7,11-Trimethyl-2,6,10-dodecatriene-1-yl]ester of acetic acid
(2E,6E)-3,7,11-Trimethyl-2,6,10-dodecatrienyl acetate
(E,E)-Farnesyl acetate
(E)-Farnesyl acetate
Farnesyl acetate, (E,E)-
trans-2-trans-6-Farnesyl acetate

Inchi: InChI=1S/C17H28O2/c1-14(2)8-6-9-15(3)10-7-11-16(4)12-13-19-17(5)18/h8,10,12H,6-7,

InchiKey: ZGIGZINMAOQWLX-NCZFFCEISA-N

Formula: C17H28O2

SMILES: CC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C

Mol. weight [g/mol]: 264.40

CAS: 4128-17-0

Physical Properties

Property code	Value	Unit	Source
gf	73.35	kJ/mol	Joback Method
hf	-316.72	kJ/mol	Joback Method
hfus	39.25	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.969		Crippen Method
mcvol	244.930	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1816.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1821.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
rinpol	1826.00		NIST Webbook

rinpol	1824.00	NIST Webbook
rinpol	1815.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1814.00	NIST Webbook
rinpol	1836.00	NIST Webbook
rinpol	1837.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	1810.00	NIST Webbook
rinpol	1826.00	NIST Webbook
rinpol	1812.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	1843.00	NIST Webbook
rinpol	1840.00	NIST Webbook
rinpol	1828.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1846.00	NIST Webbook
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rinpol	1837.00	NIST Webbook
rinpol	1839.00	NIST Webbook
rinpol	1842.00	NIST Webbook
rinpol	1842.00	NIST Webbook
rinpol	1854.00	NIST Webbook
rinpol	1818.00	NIST Webbook
rinpol	1817.00	NIST Webbook
rinpol	1844.00	NIST Webbook
rinpol	1847.00	NIST Webbook
rinpol	1824.00	NIST Webbook
rinpol	1850.00	NIST Webbook
rinpol	1812.00	NIST Webbook
ripol	2234.00	NIST Webbook
ripol	2222.00	NIST Webbook
ripol	2251.00	NIST Webbook
ripol	2265.00	NIST Webbook
ripol	2255.00	NIST Webbook
ripol	2273.00	NIST Webbook

ripol	2273.00		NIST Webbook
ripol	2242.00		NIST Webbook
ripol	2234.00		NIST Webbook
ripol	2261.00		NIST Webbook
ripol	2259.00		NIST Webbook
ripol	2257.00		NIST Webbook
ripol	2255.00		NIST Webbook
ripol	2251.00		NIST Webbook
ripol	2280.00		NIST Webbook
ripol	2276.00		NIST Webbook
ripol	2283.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2265.00		NIST Webbook
tb	676.77	K	Joback Method
tc	866.41	K	Joback Method
tf	296.39	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.60	J/mol×K	676.77	Joback Method
cpg	684.20	J/mol×K	708.38	Joback Method
cpg	700.91	J/mol×K	739.98	Joback Method
cpg	716.78	J/mol×K	771.59	Joback Method
cpg	731.87	J/mol×K	803.19	Joback Method
cpg	746.22	J/mol×K	834.80	Joback Method
cpg	759.89	J/mol×K	866.41	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	0.04	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4128170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume