Hexanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-

Other names: 2,6-Octadien-1-ol, 3,7-dimethyl-, hexanoate, (E)-
(E)-3,7-Dimethylocta-2,6-dien-1-yl n-hexanoate
Geranyl caproate
Geranyl hexanoate
Hexanoic acid, 3,7-dimethylocta-2,6-dien-1-yl ester, (E)-
Geranyl n-hexanoate
(2E)-3,7-Dimethyl-2,6-octadienyl hexanoate
Hexanoic acid, (2E)-3,7-dimethyl-2,6-octadien-1-yl ester
Hexanoic acid, (2E)-3,7-dimethyl-2,6-octadienyl ester

Inchi: InChI=1S/C16H28O2/c1-5-6-7-11-16(17)18-13-12-15(4)10-8-9-14(2)3/h9,12H,5-8,10-11,

InchiKey: ARVSCQUZFFSNKF-NTCAYCPXSA-N

Formula: C16H28O2

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

Mol. weight [g/mol]: 252.39

CAS: 10032-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-6.74	kJ/mol	Joback Method
hf	-403.51	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	60.44	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.803		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1733.00		NIST Webbook

rinpol	1727.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1718.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1755.70		NIST Webbook
rinpol	1725.00		NIST Webbook
ripol	2105.00		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2105.00		NIST Webbook
tb	649.85	K	Joback Method
tc	832.31	K	Joback Method
tf	304.16	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.54	J/mol×K	649.85	Joback Method
cpg	650.98	J/mol×K	680.26	Joback Method
cpg	667.59	J/mol×K	710.67	Joback Method
cpg	683.39	J/mol×K	741.08	Joback Method
cpg	698.43	J/mol×K	771.49	Joback Method
cpg	712.73	J/mol×K	801.90	Joback Method
cpg	726.35	J/mol×K	832.31	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10032027&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume