

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

Other names:	(2E)-3,7-Dimethyl-2,6-octadienyl pentanoate Geranyl pentanoate Geranyl valerate
Inchi:	InChI=1S/C15H26O2/c1-5-6-10-15(16)17-12-11-14(4)9-7-8-13(2)3/h8,11H,5-7,9-10,12H2
InchiKey:	CVSWGLSBJFKWMW-SDNWHVSQSA-N
Formula:	C15H26O2
SMILES:	CCCCC(=O)OCC=C(C)CCC=C(C)C
Mol. weight [g/mol]:	238.37
CAS:	10402-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-15.16	kJ/mol	Joback Method
hf	-382.87	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.412		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1625.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1633.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1658.90		NIST Webbook
rinpol	1677.00		NIST Webbook
rinpol	1658.90		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1649.00		NIST Webbook

rinpol	1642.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1641.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1983.00		NIST Webbook
tb	626.97	K	Joback Method
tc	810.82	K	Joback Method
tf	292.89	K	Joback Method
vc	0.862	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.64	J/mol×K	626.97	Joback Method
cpg	596.65	J/mol×K	657.61	Joback Method
cpg	612.84	J/mol×K	688.25	Joback Method
cpg	628.25	J/mol×K	718.90	Joback Method
cpg	642.90	J/mol×K	749.54	Joback Method
cpg	656.84	J/mol×K	780.18	Joback Method
cpg	670.10	J/mol×K	810.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10402478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rlnpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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