1,6-Octadien-3-ol, 3,7-dimethyl-, propanoate

Other names:	1,6-Octadien-3-ol, 3,7-dimethyl-, propionate
	Linalyl propionate
	Linalyl n-propionate
	Linalyl propanoate
Inchi:	InChI=1S/C13H22O2/c1-6-12(14)15-13(5,7-2)10-8-9-11(3)4/h7,9H,2,6,8,10H2,1,3-5H3
InchiKey:	WAQIIHCCEMGYKP-UHFFFAOYSA-N
Formula:	C13H22O2
SMILES:	C=CC(C)(CCC=C(C)C)OC(=O)CC
Mol. weight [g/mol]:	210.31
CAS:	144-39-8

Physical Properties

Property code	Value	Unit	Source
gf	-12.99	kJ/mol	Joback Method
hf	-332.34	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	51.76	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.631		Crippen Method
mcvol	192.870	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	1338.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1321.40		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1319.00		NIST Webbook

rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1696.00		NIST Webbook
ripol	1690.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1624.00		NIST Webbook
tb	570.62	K	Joback Method
tc	761.16	K	Joback Method
tf	290.05	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.02	J/mol×K	570.62	Joback Method
cpg	494.53	J/mol×K	602.38	Joback Method
cpg	510.14	J/mol×K	634.13	Joback Method
cpg	524.91	J/mol×K	665.89	Joback Method
cpg	538.88	J/mol×K	697.65	Joback Method
cpg	552.08	J/mol×K	729.40	Joback Method
cpg	564.56	J/mol×K	761.16	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C144398&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

Latest version available from:
https://www.chemeo.com/cid/32-592-9/1-6-Octadien-3-ol-3-7-dimethyl-propanoate.pdf
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