

2,6-Dimethyl-2,6-octadiene-1,8-diol diacetate

Other names:	Octa-2,6-diene, 1,8-diacetoxy-2,6-dimethyl-(2E,6E)-2,6-Dimethylocta-2,6-diene-1,8-diyl diacetate
Inchi:	InChI=1S/C14H22O4/c1-11(8-9-17-13(3)15)6-5-7-12(2)10-18-14(4)16/h7-8H,5-6,9-10H2
InchiKey:	PJAHPEXZWNUNLF-NFLJZBCPSA-N
Formula:	C14H22O4
SMILES:	CC(=O)OCC=C(C)CCC=C(C)COC(C)=O
Mol. weight [g/mol]:	254.32
CAS:	36052-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-257.50	kJ/mol	Joback Method
hf	-607.03	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-3.12		Crippen Method
logp	2.785		Crippen Method
mcvol	214.400	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpwl	1740.60		NIST Webbook
rinpwl	1740.60		NIST Webbook
tb	680.38	K	Joback Method
tc	872.22	K	Joback Method
tf	353.78	K	Joback Method
vc	0.830	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.21	J/molxK	680.38	Joback Method
cpg	592.19	J/molxK	712.35	Joback Method
cpg	606.40	J/molxK	744.33	Joback Method
cpg	619.85	J/molxK	776.30	Joback Method
cpg	632.57	J/molxK	808.27	Joback Method

cpg	644.59	J/mol×K	840.24	Joback Method
cpg	655.92	J/mol×K	872.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C36052536&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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