

Pentadeca-2,5E,13-triene, 7-acetoxymethyl-10-methylene-2,6,14-trimethyl

PubChem ID: [15117\(2\)10-8-12-19\(5\)14-15-22\(16-24-21\(7\)23\)20\(6\)13-9-11-18\(3\)](#)
InChI: [1S/C22H36O2/C1-17\(2\)10-8-12-19\(5\)14-15-22\(16-24-21\(7\)23\)20\(6\)13-9-11-18\(3\)](#)
InChIKey: [MVDJJPWRUBBCPLXDEDYPNTBSA-N](#)

Formula: C₂₂H₃₆O₂

SMILES: C=C(CCC=C(C)C)CCC(COC(C)=O)C(C)=CCC=C(C)C

Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	192.30	kJ/mol	Joback Method
hf	-309.56	kJ/mol	Joback Method
hfus	46.09	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.551		Crippen Method
mcvol	311.080	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinqol	2129.00		NIST Webbook
tb	787.29	K	Joback Method
tc	980.15	K	Joback Method
tf	322.02	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.23	J/molxK	787.29	Joback Method
cpg	949.35	J/molxK	819.43	Joback Method
cpg	967.52	J/molxK	851.58	Joback Method
cpg	984.81	J/molxK	883.72	Joback Method
cpg	1001.28	J/molxK	915.86	Joback Method
cpg	1017.00	J/molxK	948.01	Joback Method
cpg	1032.06	J/molxK	980.15	Joback Method

Sources

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=R604410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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