(Z)-5-tangerinol [6,10-dimethyl-(Z)-5,9-undecadienyl 2-acetate]

Other names: (Z)-6,10-dimethylundeca-5,9-dien-2-yl acetate
Inchi: InChI=1S/C15H26O2/c1-12(2)8-6-9-13(3)10-7-11-14(4)17-15(5)16/h8,10,14H,6-7,9,11H2
InchiKey: BXGLLMNDXKACMT-RAXLEYEMSA-N
Formula: C15H26O2
SMILES: CC(=O)OC(C)CCC=C(C)CCC=C(C)C
Mol. weight [g/mol]: 238.37
CAS: 3239-37-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.60	kJ/mol	Joback Method
hf	-388.15	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	57.83	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.411		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
ripol	1871.00		NIST Webbook
tb	626.53	K	Joback Method
tc	813.52	K	Joback Method
tf	277.89	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.04	J/mol×K	626.53	Joback Method
cpg	597.38	J/mol×K	657.69	Joback Method
cpg	613.87	J/mol×K	688.86	Joback Method
cpg	629.53	J/mol×K	720.02	Joback Method
cpg	644.42	J/mol×K	751.19	Joback Method
cpg	658.56	J/mol×K	782.35	Joback Method
cpg	671.98	J/mol×K	813.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3239370&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

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