(S,E)-2,5-Dimethyl-4-vinylhexa-2,5-dien-1-yl acetate

Inchi: InChI=1S/C12H18O2/c1-6-12(9(2)3)7-10(4)8-14-11(5)13/h6-7,12H,1-2,8H2,3-5H3/b10-7
InchiKey: MYZPBDIATBBLPX-OFFHKIPUSA-N
Formula: C12H18O2
SMILES: C=CC(C=C(C)COC(C)=O)C(=C)C
Mol. weight [g/mol]: 194.27
CAS: 20384-05-8

Physical Properties

Property code	Value	Unit	Source
gf	52.60	kJ/mol	Joback Method
hf	-192.59	kJ/mol	Joback Method
hfus	21.12	kJ/mol	Joback Method
hvap	49.85	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.874		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	1413.40		NIST Webbook
rinpol	1413.40		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1488.00		NIST Webbook
tb	547.09	K	Joback Method
tc	739.96	K	Joback Method
tf	245.64	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.18	J/mol×K	547.09	Joback Method
cpg	421.19	J/mol×K	579.23	Joback Method
cpg	435.43	J/mol×K	611.38	Joback Method
cpg	448.94	J/mol×K	643.52	Joback Method
cpg	461.74	J/mol×K	675.67	Joback Method

cpg	473.87	J/mol×K	707.81	Joback Method
cpg	485.35	J/mol×K	739.96	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=C20384058&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume