Vestitenone

Inchi: InChI=1S/C12H18O/c1-9-4-6-12(7-5-9)10(2)8-11(3)13/h4,8,12H,5-7H2,1-3H3/b10-8+
InchiKey: SSDLCRAPQKJETK-CSKARUKUSA-N
Formula: C12H18O
SMILES: CC(=O)C=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 178.27
CAS: 69401-36-1

Physical Properties

Property code	Value	Unit	Source
gf	37.69	kJ/mol	Joback Method
hf	-195.53	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	50.47	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.268		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
rinpol	1453.10		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1453.10		NIST Webbook
tb	555.56	K	Joback Method
tc	772.79	K	Joback Method
tf	276.55	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.81	J/mol×K	555.56	Joback Method
cpg	406.94	J/mol×K	591.77	Joback Method
cpg	423.98	J/mol×K	627.97	Joback Method
cpg	439.99	J/mol×K	664.18	Joback Method
cpg	455.01	J/mol×K	700.38	Joback Method
cpg	469.08	J/mol×K	736.59	Joback Method

cpg	482.26	J/mol×K	772.79	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=C69401361&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