2(3H)-Benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-7-(1-methylethe
[3S-(3«alpha»,3a«alpha»,6«alpha»,7«beta»,7a«bet

Other names: 2(3H)-Benzofuranone, hexahydro-7-isopropenyl-3,6-dimethyl-6-vinyl-, (all-S)-; Saussurea lactone

Inchi: InChI=1S/C15H22O2/c1-6-15(5)8-7-11-10(4)14(16)17-13(11)12(15)9(2)3/h6,10-13H,1-2,

InchiKey: LMNJALUUIMXUQQ-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: C=CC1(C)CCC2C(C)C(=O)OC2C1C(=C)C

Mol. weight [g/mol]: 234.33

CAS: 23527-07-3

Physical Properties

Property code	Value	Unit	Source
gf	90.42	kJ/mol	Joback Method
hf	-300.22	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	54.75	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.342		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	1806.30		NIST Webbook
rinpol	1806.30		NIST Webbook
tb	643.13	K	Joback Method
tc	872.16	K	Joback Method
tf	372.62	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.05	J/mol×K	643.13	Joback Method
cpg	597.18	J/mol×K	681.30	Joback Method
cpg	618.07	J/mol×K	719.47	Joback Method
cpg	637.86	J/mol×K	757.65	Joback Method
cpg	656.69	J/mol×K	795.82	Joback Method

cpg	674.69	J/mol×K	833.99	Joback Method
cpg	692.00	J/mol×K	872.16	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=C23527073&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