«beta»-Cyclodihydrocostunolide

Inchi: InChI=1S/C15H22O2/c1-9-5-4-7-15(3)8-6-11-10(2)14(16)17-13(11)12(9)15/h10-13H,1,4-
InchiKey: VVFHGZOZXJXSNR-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C1CCCC2(C)CCC3C(C)C(=O)OC3C12
Mol. weight [g/mol]: 234.33
CAS: 22387-64-0

Physical Properties

Property code	Value	Unit	Source
gf	32.73	kJ/mol	Joback Method
hf	-370.07	kJ/mol	Joback Method
hfus	22.79	kJ/mol	Joback Method
hvap	56.56	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.320		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1946.60		NIST Webbook
tb	664.73	K	Joback Method
tc	905.44	K	Joback Method
tf	422.44	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.64	J/mol×K	664.73	Joback Method
cpg	607.67	J/mol×K	704.85	Joback Method
cpg	629.35	J/mol×K	744.97	Joback Method
cpg	649.87	J/mol×K	785.09	Joback Method
cpg	669.38	J/mol×K	825.20	Joback Method
cpg	688.07	J/mol×K	865.32	Joback Method
cpg	706.09	J/mol×K	905.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22387640&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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