(5a«alpha»,9a«alpha»)-4,5,5a,6,7,8,9,9a-octahydro (Isodrimenin)

Other names: Isodrimenin
Inchi: InChI=1S/C15H22O2/c1-14(2)7-4-8-15(3)11(14)6-5-10-9-17-13(16)12(10)15/h11H,4-9H2
InchiKey: MEGPFBRAROUGQD-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CC1(C)CCCC2(C)C3=C(CCC12)COC3=O
Mol. weight [g/mol]: 234.33
CAS: 36506-91-9

Physical Properties

Property code	Value	Unit	Source
gf	0.28	kJ/mol	Joback Method
hf	-363.55	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	57.48	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.466		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	684.27	K	Joback Method
tc	935.98	K	Joback Method
tf	466.94	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.41	J/mol×K	684.27	Joback Method
cpg	599.11	J/mol×K	726.22	Joback Method
cpg	619.96	J/mol×K	768.17	Joback Method
cpg	640.32	J/mol×K	810.12	Joback Method
cpg	660.51	J/mol×K	852.08	Joback Method
cpg	680.88	J/mol×K	894.03	Joback Method

cpg	701.77	J/mol×K	935.98	Joback Method

Sources

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=C36506919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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