(3R,3aR,4aR,8aR,9aR)-3,8a-Dimethyl-5-methylene

Inchi: InChI=1S/C15H20O2/c1-9-5-4-6-15(3)8-13-11(7-12(9)15)10(2)14(16)17-13/h4,6,10-13H,
InchiKey: VHANAQXZAJSCOS-MJDBTJCESA-N
Formula: C15H20O2
SMILES: C=C1CC=CC2(C)CC3OC(=O)C(C)C3CC12
Mol. weight [g/mol]: 232.32
CAS: 66964-62-3

Physical Properties

Property code	Value	Unit	Source
gf	62.69	kJ/mol	Joback Method
hf	-312.29	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.096		Crippen Method
mcvol	188.470	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1957.40		NIST Webbook
rinpol	1957.40		NIST Webbook
tb	663.89	K	Joback Method
tc	906.87	K	Joback Method
tf	423.20	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.58	J/mol×K	663.89	Joback Method
cpg	583.52	J/mol×K	704.39	Joback Method
cpg	604.17	J/mol×K	744.88	Joback Method
cpg	623.69	J/mol×K	785.38	Joback Method
cpg	642.28	J/mol×K	825.88	Joback Method
cpg	660.09	J/mol×K	866.37	Joback Method
cpg	677.31	J/mol×K	906.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66964623&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

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