1,1,3a-Trimethyl-6-methylene-5-oxo-1,1a,2,3,3a,3b

Other names: Myli-4(15)-en-3-one
Inchi: InChI=1S/C15H20O/c1-8-10(16)7-11-14(4)6-5-9-12(13(9,2)3)15(8,11)14/h9,11-12H,1,5-7
InchiKey: ILQBQVXJORSQDH-LMCMSHIWSA-N
Formula: C15H20O
SMILES: C=C1C(=O)CC2C3(C)CCC4C(C4(C)C)C123
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	229.12	kJ/mol	Joback Method
hf	-103.99	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	48.80	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.204		Crippen Method
mcvol	176.040	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1617.00		NIST Webbook
tb	623.65	K	Joback Method
tc	863.11	K	Joback Method
tf	479.21	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.02	J/mol×K	623.65	Joback Method
cpg	538.50	J/mol×K	663.56	Joback Method
cpg	557.02	J/mol×K	703.47	Joback Method
cpg	575.07	J/mol×K	743.38	Joback Method
cpg	593.14	J/mol×K	783.29	Joback Method
cpg	611.72	J/mol×K	823.20	Joback Method
cpg	631.31	J/mol×K	863.11	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=R407704&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