1,3,3-Trimethyl-7-(5-methylcyclopenta-1,4-dien-1-yl)bicyclo[2.2.1]heptane

InChI: InChI=1S/C15H22O/c1-10-6-5-7-11(10)13-12-8-9-15(13,4)16-14(12,2)3/h6-7,12-13H,5,8-

InChIKey: DQXNTIGIDAIKGR-UHFFFAOYSA-N

Formula: C15H22O

SMILES: CC1=CCC=C1C1C2CCC1(C)OC2(C)C

Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	157.22	kJ/mol	Joback Method
hf	-182.25	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.857		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook
tb	606.67	K	Joback Method
tc	840.69	K	Joback Method
tf	398.76	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.90	J/mol×K	606.67	Joback Method
cpg	539.75	J/mol×K	645.67	Joback Method
cpg	559.32	J/mol×K	684.68	Joback Method
cpg	577.94	J/mol×K	723.68	Joback Method
cpg	595.91	J/mol×K	762.68	Joback Method
cpg	613.56	J/mol×K	801.69	Joback Method
cpg	631.20	J/mol×K	840.69	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=R407744&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