

2,6-Dimethyl-6-(4-methyl-3-pentenyl)-bicyclo[3,1,1]

Inchi:	InChI=1S/C15H26/c1-11(2)6-5-9-15(4)13-8-7-12(3)14(15)10-13/h6,12-14H,5,7-10H2,1-4
InchiKey:	KNZCEIIVAZSSPG-UHFFFAOYSA-N
Formula:	C15H26
SMILES:	CC(C)=CCCC1(C)C2CCC(C)C1C2
Mol. weight [g/mol]:	206.37

Physical Properties

Property code	Value	Unit	Source
gf	235.58	kJ/mol	Joback Method
hf	-131.50	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	47.25	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.805		Crippen Method
mvol	196.190	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1598.00		NIST Webbook
rinpol	1598.00		NIST Webbook
tb	555.29	K	Joback Method
tc	759.61	K	Joback Method
tf	287.55	K	Joback Method
vc	0.758	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.02	J/mol×K	555.29	Joback Method
cpg	538.39	J/mol×K	589.34	Joback Method
cpg	559.40	J/mol×K	623.40	Joback Method
cpg	579.20	J/mol×K	657.45	Joback Method
cpg	597.94	J/mol×K	691.51	Joback Method
cpg	615.76	J/mol×K	725.56	Joback Method
cpg	632.82	J/mol×K	759.61	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=R284105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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