

Anti-1,2,3,5,6-pentamethyl-4-methylenebicyclo[3.1.1]

Inchi:	InChI=1S/C12H18/c1-7-8(2)11(5)10(4)12(11,6)9(7)3/h10H,2H2,1,3-6H3
InchiKey:	HDCJWTTZLOHNHX-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	C=C1C(C)=C(C)C2(C)C(C)C12C
Mol. weight [g/mol]:	162.27
CAS:	20055-93-0

Physical Properties

Property code	Value	Unit	Source
gf	216.75	kJ/mol	Joback Method
hf	-16.19	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	41.30	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.555		Crippen Method
mcvol	149.620	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
tb	491.53	K	Joback Method
tc	699.09	K	Joback Method
tf	343.92	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.11	J/molxK	491.53	Joback Method
cpg	366.63	J/molxK	526.12	Joback Method
cpg	381.86	J/molxK	560.72	Joback Method
cpg	396.01	J/molxK	595.31	Joback Method
cpg	409.27	J/molxK	629.90	Joback Method
cpg	421.84	J/molxK	664.49	Joback Method
cpg	433.95	J/molxK	699.09	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=C20055930&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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