3-((1S,5S,6R)-2,6-Dimethylbicyclo[3.1.1]hept-2-en-

Inchi: InChI=1S/C12H18O/c1-9-4-5-10-8-11(9)12(10,2)6-3-7-13/h4,7,10-11H,3,5-6,8H2,1-2H3
InchiKey: PIUJKRNONSPYOP-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CC1=CCC2CC1C2(C)CCC=O
Mol. weight [g/mol]: 178.27
CAS: 203499-08-5

Physical Properties

Property code	Value	Unit	Source
gf	67.17	kJ/mol	Joback Method
hf	-195.94	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	48.52	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.958		Crippen Method
mcvol	155.490	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1356.50		NIST Webbook
tb	540.08	K	Joback Method
tc	747.77	K	Joback Method
tf	332.30	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.50	J/mol×K	540.08	Joback Method
cpg	409.64	J/mol×K	574.70	Joback Method
cpg	425.65	J/mol×K	609.31	Joback Method
cpg	440.67	J/mol×K	643.93	Joback Method
cpg	454.84	J/mol×K	678.54	Joback Method
cpg	468.29	J/mol×K	713.16	Joback Method
cpg	481.15	J/mol×K	747.77	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C203499085&Units=SI

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

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