

Bicyclo[5.1.0]octane, 8-(1-methylethylidene)-

Inchi:	InChI=1S/C11H18/c1-8(2)11-9-6-4-3-5-7-10(9)11/h9-10H,3-7H2,1-2H3
InchiKey:	RAROQJZQARUXBD-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	CC(C)=C1C2CCCCC1C2
Mol. weight [g/mol]:	150.26
CAS:	54166-47-1

Physical Properties

Property code	Value	Unit	Source
gf	175.95	kJ/mol	Joback Method
hf	-70.85	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	41.12	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.533		Crippen Method
mcvol	139.830	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1099.00		NIST Webbook
tb	479.62	K	Joback Method
tc	693.53	K	Joback Method
tf	238.97	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.33	J/mol×K	479.62	Joback Method
cpg	338.28	J/mol×K	515.27	Joback Method
cpg	356.98	J/mol×K	550.92	Joback Method
cpg	374.50	J/mol×K	586.58	Joback Method
cpg	390.93	J/mol×K	622.23	Joback Method
cpg	406.32	J/mol×K	657.88	Joback Method
cpg	420.76	J/mol×K	693.53	Joback Method

Sources

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=C54166471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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