

(5S)-5-Methyl-5-hydroxymethylbicyclo[2.2.1]hept-

Inchi:	InChI=1S/C9H14O/c1-9(6-10)5-7-2-3-8(9)4-7/h2-3,7-8,10H,4-6H2,1H3/t7?,8?,9-/m1/s1
InchiKey:	WNHHRXSVKWWRJY-AMDVSUOASA-N
Formula:	C9H14O
SMILES:	CC1(CO)CC2C=CC1C2
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
gf	14.24	kJ/mol	Joback Method
hf	-189.20	kJ/mol	Joback Method
hfus	13.32	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.581		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	1089.00		NIST Webbook
tb	509.98	K	Joback Method
tc	707.86	K	Joback Method
tf	304.79	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.66	J/molxK	509.98	Joback Method
cpg	303.65	J/molxK	542.96	Joback Method
cpg	316.63	J/molxK	575.94	Joback Method
cpg	328.73	J/molxK	608.92	Joback Method
cpg	340.07	J/molxK	641.90	Joback Method
cpg	350.75	J/molxK	674.88	Joback Method
cpg	360.90	J/molxK	707.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R557443&Units=SI
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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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