

cis-Bicyclo[3.2.0]heptane

Other names:	cis-Bicyclo[3.2.0]heptane
Inchi:	InChI=1S/C7H8O/c8-7-4-5-2-1-3-6(5)7/h1-2,5-6H,3-4H2
InchiKey:	LNLLHUHPGPKRBM-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	O=C1CC2C=CCC12
Mol. weight [g/mol]:	108.14

Physical Properties

Property code	Value	Unit	Source
hfus	8.79	kJ/mol	Joback Method
logp	1.151		Crippen Method
mcvol	85.040	ml/mol	McGowan Method
rinpol	787.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.45	J/mol×K	444.29	Joback Method
cpg	190.19	J/mol×K	482.08	Joback Method
cpg	203.08	J/mol×K	519.86	Joback Method
cpg	215.13	J/mol×K	557.65	Joback Method
cpg	226.41	J/mol×K	595.44	Joback Method
cpg	236.95	J/mol×K	633.22	Joback Method
cpg	246.79	J/mol×K	671.01	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13173096&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/47-684-1/cis-Bicyclo-3-2-0-heptane.pdf>

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