

1-methyl-1-(2,3-methylene)propyl-cyclopropane

Inchi:	InChI=1S/C8H14/c1-8(4-5-8)6-7-2-3-7/h7H,2-6H2,1H3
InchiKey:	DYIGSOOHRXOBCZ-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC1(CC2CC2)CC1
Mol. weight [g/mol]:	110.20

Physical Properties

Property code	Value	Unit	Source
gf	132.49	kJ/mol	Joback Method
hf	-47.61	kJ/mol	Joback Method
hfus	6.45	kJ/mol	Joback Method
hvap	32.08	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.587		Crippen Method
mcvol	101.860	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	781.80		NIST Webbook
rinpol	781.80		NIST Webbook
rinpol	778.00		NIST Webbook
tb	396.16	K	Joback Method
tc	598.18	K	Joback Method
tf	239.70	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.76	J/molxK	396.16	Joback Method
cpg	218.98	J/molxK	429.83	Joback Method
cpg	234.75	J/molxK	463.50	Joback Method
cpg	249.22	J/molxK	497.17	Joback Method
cpg	262.50	J/molxK	530.84	Joback Method
cpg	274.75	J/molxK	564.51	Joback Method
cpg	286.09	J/molxK	598.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R137178&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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