1-methyl-cis-2-(1-cis-propenyl)-cyclopropane

Inchi: InChI=1S/C7H12/c1-3-4-7-5-6(7)2/h3-4,6-7H,5H2,1-2H3/b4-3-/t6-,7+/m1/s1
InchiKey: LNAVSCYUHFMDNS-FKCQFORESA-N
Formula: C7H12
SMILES: CC=CC1CC1C
Mol. weight [g/mol]: 96.17

Physical Properties

Property code	Value	Unit	Source
gf	141.32	kJ/mol	Joback Method
hf	-18.13	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	30.74	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.219		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	723.90		NIST Webbook
rinpol	725.50		NIST Webbook
rinpol	725.50		NIST Webbook
rinpol	723.70		NIST Webbook
tb	365.79	K	Joback Method
tc	552.98	K	Joback Method
tf	177.27	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.81	J/mol×K	365.79	Joback Method
cpg	177.37	J/mol×K	396.99	Joback Method
cpg	190.19	J/mol×K	428.19	Joback Method
cpg	202.31	J/mol×K	459.38	Joback Method
cpg	213.75	J/mol×K	490.58	Joback Method
cpg	224.57	J/mol×K	521.78	Joback Method

cpg	234.79	J/mol×K	552.98	Joback Method
dvisc	0.0003994	Pa×s	177.27	Joback Method
dvisc	0.0003421	Pa×s	208.69	Joback Method
dvisc	0.0003051	Pa×s	240.11	Joback Method
dvisc	0.0002795	Pa×s	271.53	Joback Method
dvisc	0.0002607	Pa×s	302.95	Joback Method
dvisc	0.0002464	Pa×s	334.37	Joback Method
dvisc	0.0002351	Pa×s	365.79	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=R137252&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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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