cis-2-butenyl-cyclopropane

Inchi: InChI=1S/C7H12/c1-2-3-4-7-5-6-7/h2-3,7H,4-6H2,1H3/b3-2-
InchiKey: HFWBELFXCMGIGS-IHWYPQMZSA-N
Formula: C7H12
SMILES: CC=CCC1CC1
Mol. weight [g/mol]: 96.17

Physical Properties

Property code	Value	Unit	Source
gf	149.03	kJ/mol	Joback Method
hf	2.21	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	31.05	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.363		Crippen Method
mcvol	94.330	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	723.60		NIST Webbook
rinpol	725.00		NIST Webbook
rinpol	721.40		NIST Webbook
tb	370.46	K	Joback Method
tc	558.31	K	Joback Method
tf	181.51	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.59	J/mol×K	370.46	Joback Method
cpg	176.97	J/mol×K	401.77	Joback Method
cpg	189.56	J/mol×K	433.08	Joback Method
cpg	201.42	J/mol×K	464.39	Joback Method
cpg	212.58	J/mol×K	495.70	Joback Method
cpg	223.08	J/mol×K	527.00	Joback Method
cpg	232.96	J/mol×K	558.31	Joback Method

dvisc	0.0008992	Pa×s	181.51	Joback Method
dvisc	0.0006335	Pa×s	213.00	Joback Method
dvisc	0.0004884	Pa×s	244.49	Joback Method
dvisc	0.0003996	Pa×s	275.99	Joback Method
dvisc	0.0003407	Pa×s	307.48	Joback Method
dvisc	0.0002992	Pa×s	338.97	Joback Method
dvisc	0.0002686	Pa×s	370.46	Joback Method

Sources

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=R137841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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