

1-(1-Ethenyl)-cis-2-butyl-cyclopropane

Inchi:	InChI=1S/C9H16/c1-3-5-6-9-7-8(9)4-2/h4,8-9H,2-3,5-7H2,1H3/t8-,9+/m1/s1
InchiKey:	OROUOQQBLPHIHQ-BDAKNGLRSA-N
Formula:	C9H16
SMILES:	C=CC1CC1CCCC
Mol. weight [g/mol]:	124.22

Physical Properties

Property code	Value	Unit	Source
gf	165.78	kJ/mol	Joback Method
hf	-51.20	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	34.56	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.999		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	889.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	886.30		NIST Webbook
tb	404.07	K	Joback Method
tc	583.81	K	Joback Method
tf	203.13	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.09	J/molxK	404.07	Joback Method
cpg	257.45	J/molxK	434.03	Joback Method
cpg	272.06	J/molxK	463.98	Joback Method
cpg	285.97	J/molxK	493.94	Joback Method
cpg	299.19	J/molxK	523.90	Joback Method
cpg	311.76	J/molxK	553.85	Joback Method
cpg	323.71	J/molxK	583.81	Joback Method

dvisc	0.0007831	Paxs	203.13	Joback Method
dvisc	0.0006226	Paxs	236.62	Joback Method
dvisc	0.0005239	Paxs	270.11	Joback Method
dvisc	0.0004580	Paxs	303.60	Joback Method
dvisc	0.0004112	Paxs	337.09	Joback Method
dvisc	0.0003765	Paxs	370.58	Joback Method
dvisc	0.0003498	Paxs	404.07	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=R136922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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