1-(1-Ethenyl)-trans-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-RKDXNWHRSA-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	862.60		NIST Webbook
rinpol	866.50		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/mol×K	404.07	Joback Method
cpg	257.45	J/mol×K	434.03	Joback Method
cpg	272.06	J/mol×K	463.98	Joback Method
cpg	285.97	J/mol×K	493.94	Joback Method
cpg	299.19	J/mol×K	523.90	Joback Method
cpg	311.76	J/mol×K	553.85	Joback Method
cpg	323.71	J/mol×K	583.81	Joback Method
dvisc	0.0007831	Pa×s	203.13	Joback Method

dvisc	0.0006226	Pa×s	236.62	Joback Method
dvisc	0.0005239	Pa×s	270.11	Joback Method
dvisc	0.0004580	Pa×s	303.60	Joback Method
dvisc	0.0004112	Pa×s	337.09	Joback Method
dvisc	0.0003765	Pa×s	370.58	Joback Method
dvisc	0.0003498	Pa×s	404.07	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=R136977&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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