

1-Ethyl-trans-2-butyl-cyclopropane

Inchi:	InChI=1S/C9H18/c1-3-5-6-9-7-8(9)4-2/h8-9H,3-7H2,1-2H3/t8-,9-/m1/s1
InchiKey:	RNEGJSGKJQQNEI-RKDXNWHRSA-N
Formula:	C9H18
SMILES:	CCCCC1CC1CC
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	77.94	kJ/mol	Joback Method
hf	-176.63	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	35.23	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	860.20		NIST Webbook
rinpol	857.50		NIST Webbook
rinpol	858.80		NIST Webbook
rinpol	860.20		NIST Webbook
tb	407.39	K	Joback Method
tc	583.43	K	Joback Method
tf	204.89	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.60	J/molxK	407.39	Joback Method
cpg	273.45	J/molxK	436.73	Joback Method
cpg	288.59	J/molxK	466.07	Joback Method
cpg	303.05	J/molxK	495.41	Joback Method
cpg	316.85	J/molxK	524.75	Joback Method
cpg	330.01	J/molxK	554.09	Joback Method

cpg	342.57	J/molxK	583.43	Joback Method
dvisc	0.0009405	Paxs	204.89	Joback Method
dvisc	0.0007164	Paxs	238.64	Joback Method
dvisc	0.0005837	Paxs	272.39	Joback Method
dvisc	0.0004976	Paxs	306.14	Joback Method
dvisc	0.0004379	Paxs	339.89	Joback Method
dvisc	0.0003943	Paxs	373.64	Joback Method
dvisc	0.0003613	Paxs	407.39	Joback Method

Sources

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=R137143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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