1-ethyl-cis-2-butylcyclopropane

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-BDAKNGLRSA-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	888.00		NIST Webbook
rinpol	890.50		NIST Webbook
rinpol	890.50		NIST Webbook
rinpol	886.80		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/mol×K	407.39	Joback Method
cpg	330.01	J/mol×K	554.09	Joback Method
cpg	316.85	J/mol×K	524.75	Joback Method
cpg	303.05	J/mol×K	495.41	Joback Method
cpg	288.59	J/mol×K	466.07	Joback Method
cpg	273.45	J/mol×K	436.73	Joback Method

cpg	342.57	J/mol×K	583.43	Joback Method
dvisc	0.0003613	Pa×s	407.39	Joback Method
dvisc	0.0003943	Pa×s	373.64	Joback Method
dvisc	0.0004379	Pa×s	339.89	Joback Method
dvisc	0.0004976	Pa×s	306.14	Joback Method
dvisc	0.0005837	Pa×s	272.39	Joback Method
dvisc	0.0007164	Pa×s	238.64	Joback Method
dvisc	0.0009405	Pa×s	204.89	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R136744&Units=SI
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

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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