1,1-dimethyl-2-butyl-cyclopropane

Inchi: InChI=1S/C9H18/c1-4-5-6-8-7-9(8,2)3/h8H,4-7H2,1-3H3
InchiKey: DNSANEYRJQIXEM-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCCCC1CC1(C)C
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	72.45	kJ/mol	Joback Method
hf	-161.39	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	34.08	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	822.60		NIST Webbook
rinpol	822.60		NIST Webbook
tb	407.63	K	Joback Method
tc	591.38	K	Joback Method
tf	228.79	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.42	J/mol×K	407.63	Joback Method
cpg	274.99	J/mol×K	438.26	Joback Method
cpg	290.52	J/mol×K	468.88	Joback Method
cpg	305.09	J/mol×K	499.51	Joback Method
cpg	318.79	J/mol×K	530.13	Joback Method
cpg	331.69	J/mol×K	560.76	Joback Method
cpg	343.88	J/mol×K	591.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136893&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
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