

1,1,2-trimethyl-2-propyl-cyclopropane

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H18/c1-5-6-9(4)7-8(9,2)3/h5-7H2,1-4H3

OONRHRYPMIFDCP-UHFFFAOYSA-N

C9H18

CCCC1(C)CC1(C)C

126.24

Physical Properties

Property code	Value	Unit	Source
gf	66.96	kJ/mol	Joback Method
hf	-146.15	kJ/mol	Joback Method
hfus	5.68	kJ/mol	Joback Method
hvap	32.93	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
rinpol	805.50		NIST Webbook
rinpol	814.50		NIST Webbook
rinpol	805.50		NIST Webbook
tb	407.87	K	Joback Method
tc	599.83	K	Joback Method
tf	252.69	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.25	J/mol×K	407.87	Joback Method
cpg	276.55	J/mol×K	439.86	Joback Method
cpg	292.45	J/mol×K	471.86	Joback Method
cpg	307.09	J/mol×K	503.85	Joback Method
cpg	320.61	J/mol×K	535.84	Joback Method
cpg	333.17	J/mol×K	567.83	Joback Method
cpg	344.93	J/mol×K	599.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136888&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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