

1-Methyl-3-(1-methylethyl)cyclopentane, isomer # 1

Inchi:	InChI=1S/C9H18/c1-7(2)9-5-4-8(3)6-9/h7-9H,4-6H2,1-3H3
InchiKey:	CDTDMKCVKCGRPD-UHFFFAOYSA-N
Formula:	C9H18
SMILES:	CC1CCC(C(C)C)C1
Mol. weight [g/mol]:	126.24

Physical Properties

Property code	Value	Unit	Source
gf	51.30	kJ/mol	Joback Method
hf	-194.23	kJ/mol	Joback Method
hfus	10.55	kJ/mol	Joback Method
hvap	35.19	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	3.079		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	867.00		NIST Webbook
tb	415.49	K	Joback Method
tc	610.70	K	Joback Method
tf	182.85	K	Joback Method
vc	0.473	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.75	J/molxK	415.49	Joback Method
cpg	274.05	J/molxK	448.03	Joback Method
cpg	291.51	J/molxK	480.56	Joback Method
cpg	308.15	J/molxK	513.10	Joback Method
cpg	323.99	J/molxK	545.63	Joback Method
cpg	339.06	J/molxK	578.17	Joback Method
cpg	353.37	J/molxK	610.70	Joback Method
dvisc	0.0039722	Paxs	182.85	Joback Method
dvisc	0.0017463	Paxs	221.62	Joback Method

dvisc	0.0009806	Paxs	260.40	Joback Method
dvisc	0.0006395	Paxs	299.17	Joback Method
dvisc	0.0004600	Paxs	337.94	Joback Method
dvisc	0.0003541	Paxs	376.72	Joback Method
dvisc	0.0002863	Paxs	415.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R589376&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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