1-Methylpentyl cyclopropane

Other names: 2-Cyclopropylhexane
Inchi: InChI=1S/C9H18/c1-3-4-5-8(2)9-6-7-9/h8-9H,3-7H2,1-2H3
InchiKey: IYZQDBIQGSJSEX-UHFFFAOYSA-N
Formula: C9H18
SMILES: CCCCC(C)C1CC1
Mol. weight [g/mol]: 126.24
CAS: 6976-28-9

Physical Properties

Property code	Value	Unit	Source
chl	-5648.00	kJ/mol	NIST Webbook
gf	83.21	kJ/mol	Joback Method
hf	-161.57	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	35.15	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	416.10 ± 0.10	K	NIST Webbook
tc	592.25	K	Joback Method
tf	175.11 ± 0.20	K	NIST Webbook
tf	175.16 ± 0.10	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.65	J/mol×K	411.62	Joback Method
cpg	330.52	J/mol×K	562.15	Joback Method
cpg	317.38	J/mol×K	532.04	Joback Method
cpg	303.55	J/mol×K	501.94	Joback Method
cpg	289.01	J/mol×K	471.83	Joback Method
cpg	273.72	J/mol×K	441.73	Joback Method

cpg	343.00	J/mol×K	592.25	Joback Method
dvisc	0.0003688	Pa×s	411.62	Joback Method
dvisc	0.0004326	Pa×s	375.37	Joback Method
dvisc	0.0005250	Pa×s	339.12	Joback Method
dvisc	0.0006674	Pa×s	302.88	Joback Method
dvisc	0.0009056	Pa×s	266.63	Joback Method
dvisc	0.0013526	Pa×s	230.38	Joback Method
dvisc	0.0023468	Pa×s	194.13	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6976289&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

chl: Standard liquid enthalpy of combustion
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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