

(3-Methyl)-hexyl-cyclopropane

Inchi:

InChI=1S/C10H20/c1-3-4-9(2)5-6-10-7-8-10/h9-10H,3-8H2,1-2H3

InchiKey:

GIMQASNKLCRRKW-UHFFFAOYSA-N

Formula:

C10H20

SMILES:

CCCC(C)CCC1CC1

Mol. weight [g/mol]:

140.27

Physical Properties

Property code	Value	Unit	Source
gf	91.63	kJ/mol	Joback Method
hf	-182.21	kJ/mol	Joback Method
hfus	16.27	kJ/mol	Joback Method
hvap	37.38	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	975.09		NIST Webbook
rinpol	975.23		NIST Webbook
rinpol	973.15		NIST Webbook
rinpol	978.96		NIST Webbook
rinpol	977.35		NIST Webbook
rinpol	975.09		NIST Webbook
rinpol	975.09		NIST Webbook
tb	434.50	K	Joback Method
tc	613.84	K	Joback Method
tf	205.40	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.01	J/mol×K	434.50	Joback Method
cpg	317.97	J/mol×K	464.39	Joback Method
cpg	334.12	J/mol×K	494.28	Joback Method

cpg	349.48	J/mol×K	524.17	Joback Method
cpg	364.10	J/mol×K	554.06	Joback Method
cpg	378.01	J/mol×K	583.95	Joback Method
cpg	391.23	J/mol×K	613.84	Joback Method
dvisc	0.0027890	Pa×s	205.40	Joback Method
dvisc	0.0015449	Pa×s	243.58	Joback Method
dvisc	0.0010044	Pa×s	281.77	Joback Method
dvisc	0.0007236	Pa×s	319.95	Joback Method
dvisc	0.0005591	Pa×s	358.13	Joback Method
dvisc	0.0004540	Pa×s	396.32	Joback Method
dvisc	0.0003824	Pa×s	434.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R136828&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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