1-Methylbutylcyclopropane

Other names: 1-Methylbutylcyclopropane
Inchi: InChI=1S/C8H16/c1-3-4-7(2)8-5-6-8/h7-8H,3-6H2,1-2H3
InchiKey: HDRPKFBKHPJRQK-UHFFFAOYSA-N
Formula: C8H16
SMILES: CCCC(C)C1CC1
Mol. weight [g/mol]: 112.22

Physical Properties

Property code	Value	Unit	Source
af	0.3267		Cheméo Relay (1.0)
gf	74.79	kJ/mol	Joback Method
hf	-90.64	kJ/mol	Cheméo Relay (1.0)
hfus	11.09	kJ/mol	Joback Method
hvap	38.41	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-4.74		Cheméo Relay (1.0)
logp	2.833		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
tb	390.89 ± 0.10	K	NIST Webbook
tc	580.95	K	Cheméo Relay (1.0)
tf	149.99	K	Cheméo Relay (1.0)
vc	0.415	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.39	J/mol×K	388.74	Joback Method
cpg	296.23	J/mol×K	570.46	Joback Method
cpg	284.58	J/mol×K	540.17	Joback Method
cpg	272.31	J/mol×K	509.88	Joback Method
cpg	259.38	J/mol×K	479.60	Joback Method
cpg	245.77	J/mol×K	449.31	Joback Method
cpg	231.45	J/mol×K	419.03	Joback Method

dvisc	0.0005954	Pa×s	285.80	Joback Method
dvisc	0.0003461	Pa×s	388.74	Joback Method
dvisc	0.0004004	Pa×s	354.43	Joback Method
dvisc	0.0004780	Pa×s	320.11	Joback Method
dvisc	0.0018874	Pa×s	182.86	Joback Method
dvisc	0.0007875	Pa×s	251.49	Joback Method
dvisc	0.0011378	Pa×s	217.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5458162&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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