

5-methyl-2-hexene

Inchi:	InChI=1S/C7H14/c1-4-5-6-7(2)3/h4-5,7H,6H2,1-3H3/b5-4+
InchiKey:	GHBKCPRDHLITSE-SNAWJCMRSA-N
Formula:	C7H14
SMILES:	CC=CCC(C)C
Mol. weight [g/mol]:	98.19

Physical Properties

Property code	Value	Unit	Source
gf	85.84	kJ/mol	Joback Method
hf	-75.87	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	30.75	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.609		Crippen Method
mcvol	105.190	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	658.40		NIST Webbook
tb	363.28	K	Joback Method
tc	539.72	K	Joback Method
tf	148.57	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.16	J/mol×K	363.28	Joback Method
cpg	192.22	J/mol×K	392.69	Joback Method
cpg	203.76	J/mol×K	422.09	Joback Method
cpg	214.79	J/mol×K	451.50	Joback Method
cpg	225.33	J/mol×K	480.91	Joback Method
cpg	235.39	J/mol×K	510.31	Joback Method
cpg	245.01	J/mol×K	539.72	Joback Method
dvisc	0.0095853	Pa×s	148.57	Joback Method
dvisc	0.0026515	Pa×s	184.35	Joback Method

dvisc	0.0011138	Pa×s	220.14	Joback Method
dvisc	0.0005963	Pa×s	255.92	Joback Method
dvisc	0.0003722	Pa×s	291.71	Joback Method
dvisc	0.0002575	Pa×s	327.50	Joback Method
dvisc	0.0001915	Pa×s	363.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R306280&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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