

Hexane, 1-chloro-2-methyl

Inchi:	InChI=1S/C7H15Cl/c1-3-4-5-7(2)6-8/h7H,3-6H2,1-2H3
InchiKey:	VVROFNMTCHTDES-UHFFFAOYSA-N
Formula:	C7H15Cl
SMILES:	CCCCC(C)CCl
Mol. weight [g/mol]:	134.65

Physical Properties

Property code	Value	Unit	Source
gf	-6.31	kJ/mol	Joback Method
hf	-208.83	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	35.17	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	3.051		Crippen Method
mcvol	121.730	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	921.00		NIST Webbook
tb	396.55	K	Joback Method
tc	572.19	K	Joback Method
tf	183.57	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.17	J/mol×K	396.55	Joback Method
cpg	235.16	J/mol×K	425.82	Joback Method
cpg	246.67	J/mol×K	455.10	Joback Method
cpg	257.72	J/mol×K	484.37	Joback Method
cpg	268.31	J/mol×K	513.64	Joback Method
cpg	278.47	J/mol×K	542.91	Joback Method
cpg	288.19	J/mol×K	572.19	Joback Method

dvisc	0.0087444	Paxs	183.57	Joback Method
dvisc	0.0030894	Paxs	219.07	Joback Method
dvisc	0.0014589	Paxs	254.56	Joback Method
dvisc	0.0008278	Paxs	290.06	Joback Method
dvisc	0.0005315	Paxs	325.56	Joback Method
dvisc	0.0003723	Paxs	361.05	Joback Method
dvisc	0.0002780	Paxs	396.55	Joback Method

Sources

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=R116077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/60-224-6/Hexane-1-chloro-2-methyl.pdf>

Generated by Cheméo on 2024-04-20 04:22:24.55530729 +0000 UTC m=+15876193.475884603.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.