

1-Hexanol, 4-methyl-, (S)-

Inchi:	InChI=1S/C7H16O/c1-3-7(2)5-4-6-8/h7-8H,3-6H2,1-2H3/t7-/m1/s1
InchiKey:	YNPVNLWKVZZBTM-SSDOTTSWSA-N
Formula:	C7H16O
SMILES:	CCC(C)CCCO
Mol. weight [g/mol]:	116.20
CAS:	1767-46-0

Physical Properties

Property code	Value	Unit	Source
gf	-131.20	kJ/mol	Joback Method
hf	-345.32	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.805		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
tb	445.15 ± 2.00	K	NIST Webbook
tc	615.06	K	Joback Method
tf	214.47	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.92	J/molxK	451.30	Joback Method
cpg	258.79	J/molxK	478.59	Joback Method
cpg	269.25	J/molxK	505.89	Joback Method
cpg	279.32	J/molxK	533.18	Joback Method
cpg	289.00	J/molxK	560.47	Joback Method
cpg	298.30	J/molxK	587.77	Joback Method
cpg	307.23	J/molxK	615.06	Joback Method
dvisc	0.1594974	Paxs	214.47	Joback Method
dvisc	0.0221021	Paxs	253.94	Joback Method

dvisc	0.0052125	Paxs	293.41	Joback Method
dvisc	0.0017316	Paxs	332.88	Joback Method
dvisc	0.0007266	Paxs	372.36	Joback Method
dvisc	0.0003601	Paxs	411.83	Joback Method
dvisc	0.0002018	Paxs	451.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1767460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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