(S)-(+)-3-methylhexane

Inchi: InChI=1S/C7H16/c1-4-6-7(3)5-2/h7H,4-6H2,1-3H3/t7-/m1/s1
InchiKey: VLJXXKKOSFGPHI-SSDOTTSWSA-N
Formula: C7H16
SMILES: CCCC(C)CC
Mol. weight [g/mol]: 100.20
CAS: 6131-24-4

Physical Properties

Property code	Value	Unit	Source
gf	5.62	kJ/mol	Joback Method
hf	-193.09	kJ/mol	Joback Method
hfus	10.36	kJ/mol	Joback Method
hvap	30.79	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.833		Crippen Method
mcvol	109.490	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	359.12	K	Joback Method
tc	526.54	K	Joback Method
tf	153.65	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.02	J/mol×K	359.12	Joback Method
cpg	206.19	J/mol×K	387.02	Joback Method
cpg	217.92	J/mol×K	414.93	Joback Method
cpg	229.23	J/mol×K	442.83	Joback Method
cpg	240.13	J/mol×K	470.73	Joback Method
cpg	250.62	J/mol×K	498.63	Joback Method
cpg	260.72	J/mol×K	526.54	Joback Method
dvisc	0.0099972	Pa×s	153.65	Joback Method
dvisc	0.0030264	Pa×s	187.90	Joback Method

dvisc	0.0013243	Pa×s	222.14	Joback Method
dvisc	0.0007226	Pa×s	256.38	Joback Method
dvisc	0.0004548	Pa×s	290.63	Joback Method
dvisc	0.0003156	Pa×s	324.88	Joback Method
dvisc	0.0002348	Pa×s	359.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6131244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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