2-Hexanol, (S)-

Other names: (S)-(+)-2-Hexanol
Inchi: InChI=1S/C6H14O/c1-3-4-5-6(2)7/h6-7H,3-5H2,1-2H3/t6-/m1/s1
InchiKey: QNVRIHYSUZMSGM-ZCFIWIBFSA-N
Formula: C6H14O
SMILES: CCCCC(C)O
Mol. weight [g/mol]: 102.17
CAS: 52019-78-0

Physical Properties

Property code	Value	Unit	Source
gf	-139.62	kJ/mol	Joback Method
hf	-324.68	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	45.24	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.557		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
tb	411.20	K	NIST Webbook
tc	592.97	K	Joback Method
tf	203.20	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.74	J/mol×K	428.42	Joback Method
cpg	253.18	J/mol×K	565.55	Joback Method
cpg	244.78	J/mol×K	538.12	Joback Method
cpg	236.05	J/mol×K	510.70	Joback Method
cpg	226.97	J/mol×K	483.27	Joback Method
cpg	217.54	J/mol×K	455.85	Joback Method
cpg	261.25	J/mol×K	592.97	Joback Method
dvisc	0.0002400	Pa×s	428.42	Joback Method

dvisc	0.0004330	Pa×s	390.88	Joback Method
dvisc	0.0008856	Pa×s	353.35	Joback Method
dvisc	0.0021472	Pa×s	315.81	Joback Method
dvisc	0.0066108	Pa×s	278.27	Joback Method
dvisc	0.0289027	Pa×s	240.74	Joback Method
dvisc	0.2179366	Pa×s	203.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.65192e+01
Coeff. B	-4.23210e+03
Coeff. C	-5.55890e+01
Temperature range (K), min.	316.32
Temperature range (K), max.	433.19

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=C52019780&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume