3-Hexene

Other names: hex-3-ene
Inchi: InChI=1S/C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3
InchiKey: ZQDPJFUHLCOCRG-UHFFFAOYSA-N
Formula: C6H12
SMILES: CCC=CCC
Mol. weight [g/mol]: 84.16
CAS: 592-47-2

Physical Properties

Property code	Value	Unit	Source
gf	79.86	kJ/mol	Joback Method
hf	-49.95	kJ/mol	Joback Method
hfus	11.50	kJ/mol	Joback Method
hvap	28.91	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.363		Crippen Method
mcvol	91.100	ml/mol	McGowan Method
pc	3339.00 ± 20.00	kPa	NIST Webbook
rhoc	239.01 ± 8.42	kg/m3	NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	602.00		NIST Webbook
tb	340.40 ± 1.00	K	NIST Webbook
tb	339.95 ± 0.60	K	NIST Webbook
tb	339.85 ± 0.40	K	NIST Webbook
tb	339.90 ± 0.40	K	NIST Webbook
tb	339.79 ± 0.30	K	NIST Webbook
tb	339.76 ± 0.30	K	NIST Webbook
tc	502.25 ± 0.10	K	NIST Webbook
tf	152.30	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.03	J/mol×K	340.84	Joback Method
cpg	155.37	J/mol×K	369.56	Joback Method
cpg	165.27	J/mol×K	398.29	Joback Method
cpg	174.75	J/mol×K	427.01	Joback Method
cpg	183.82	J/mol×K	455.74	Joback Method
cpg	192.49	J/mol×K	484.46	Joback Method
cpg	200.78	J/mol×K	513.19	Joback Method
dvisc	0.0040974	Pa×s	152.30	Joback Method
dvisc	0.0015745	Pa×s	183.72	Joback Method
dvisc	0.0008000	Pa×s	215.15	Joback Method
dvisc	0.0004831	Pa×s	246.57	Joback Method
dvisc	0.0003269	Pa×s	277.99	Joback Method
dvisc	0.0002395	Pa×s	309.42	Joback Method
dvisc	0.0001858	Pa×s	340.84	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48507e+01
Coeff. B	-3.11365e+03
Coeff. C	-3.56560e+01
Temperature range (K), min.	249.46
Temperature range (K), max.	362.06

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=C592472&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

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
rhoc:	Critical density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume