3-Methyl-1-hexyne

Other names: 1-Hexyne, 3-methyl-
Inchi: InChI=1S/C7H12/c1-4-6-7(3)5-2/h2,7H,4,6H2,1,3H3
InchiKey: OPZULQHRFNTFFZ-UHFFFAOYSA-N
Formula: C7H12
SMILES: C#CC(C)CCC
Mol. weight [g/mol]: 96.17
CAS: 40276-93-5

Physical Properties

Property code	Value	Unit	Source
gf	228.69	kJ/mol	Joback Method
hf	98.81	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	30.65	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
tb	349.24	K	Joback Method
tc	528.78	K	Joback Method
tf	200.62	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.87	J/mol×K	349.24	Joback Method
cpg	182.56	J/mol×K	379.16	Joback Method
cpg	192.80	J/mol×K	409.09	Joback Method
cpg	202.59	J/mol×K	439.01	Joback Method
cpg	211.96	J/mol×K	468.93	Joback Method
cpg	220.92	J/mol×K	498.86	Joback Method

cpg	229.49	J/mol×K	528.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38410e+01
Coeff. B	-2.78779e+03
Coeff. C	-5.58750e+01
Temperature range (K), min.	261.56
Temperature range (K), max.	382.71

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=417
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40276935&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
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

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