3-Hexyne, 2-methyl-

Inchi: InChI=1S/C7H12/c1-4-5-6-7(2)3/h7H,4H2,1-3H3
InchiKey: POBOUPFSQKXZFZ-UHFFFAOYSA-N
Formula: C7H12
SMILES: CCC#CC(C)C
Mol. weight [g/mol]: 96.17
CAS: 36566-80-0

Physical Properties

Property code	Value	Unit	Source
gf	208.42	kJ/mol	Joback Method
hf	79.21	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	32.94	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.056		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
tb	367.65 ± 2.00	K	NIST Webbook
tb	367.85 ± 2.00	K	NIST Webbook
tb	368.35 ± 0.50	K	NIST Webbook
tc	561.09	K	Joback Method
tf	156.45 ± 0.40	K	NIST Webbook
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.85	J/mol×K	368.12	Joback Method
cpg	182.83	J/mol×K	400.28	Joback Method
cpg	193.38	J/mol×K	432.44	Joback Method
cpg	203.51	J/mol×K	464.60	Joback Method
cpg	213.23	J/mol×K	496.76	Joback Method

cpg	222.56	J/mol×K	528.92	Joback Method
cpg	231.49	J/mol×K	561.09	Joback Method

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol422.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36566800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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