2-Heptyne

Other names:	1-METHYL-2-BUTYLACETYLENE
	hept-2-yne
	n-C4H9C«equiv»CCH3
	n-C4H9CÂ«equivÂ»CCH3
Inchi:	InChI=1S/C7H12/c1-3-5-7-6-4-2/h3,5,7H2,1-2H3
InchiKey:	AMSFEMSYKQQCHL-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC#CCCCC
Mol. weight [g/mol]:	96.17
CAS:	1119-65-9

Physical Properties

Property code	Value	Unit	Source
gf	210.86	kJ/mol	Joback Method
hf	84.80 ± 2.20	kJ/mol	NIST Webbook
hfus	17.01	kJ/mol	Joback Method
hvap	33.33	kJ/mol	Joback Method
ie	9.33 ± 0.01	eV	NIST Webbook
ie	9.18	eV	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.200		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	746.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	766.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	747.00		NIST Webbook
rinpol	743.00		NIST Webbook
ripol	965.00		NIST Webbook

ripol	964.00		NIST Webbook
ripol	964.00		NIST Webbook
ripol	978.30		NIST Webbook
tb	385.62 ± 0.60	K	NIST Webbook
tb	383.90 ± 1.00	K	NIST Webbook
tb	385.40 ± 1.50	K	NIST Webbook
tb	112.47 ± 0.20	K	NIST Webbook
tb	366.15	K	NIST Webbook
tb	385.65 ± 2.00	K	NIST Webbook
tb	385.15 ± 2.00	K	NIST Webbook
tb	385.20	K	NIST Webbook
tb	385.15 ± 1.00	K	NIST Webbook
tc	556.83	K	Joback Method
tf	274.75	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.96	J/mol×K	368.56	Joback Method
cpg	182.57	J/mol×K	399.94	Joback Method
cpg	192.78	J/mol×K	431.32	Joback Method
cpg	202.60	J/mol×K	462.70	Joback Method
cpg	212.03	J/mol×K	494.08	Joback Method
cpg	221.10	J/mol×K	525.45	Joback Method
cpg	229.80	J/mol×K	556.83	Joback Method
hvapt	38.60	kJ/mol	365.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39871e+01
Coeff. B	-3.07825e+03
Coeff. C	-5.65840e+01
Temperature range (K), min.	281.28
Temperature range (K), max.	411.40

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.41860e+01
Coeff. B	-7.28304e+03
Coeff. C	-8.63386e+00
Coeff. D	5.02284e-06
Temperature range (K), min.	330.15
Temperature range (K), max.	386.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol415.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119659&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=415
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume