

1-Hepten-3-yne

Inchi:	InChI=1S/C7H10/c1-3-5-7-6-4-2/h3H,1,4,6H2,2H3
InchiKey:	NKFFXBOEFRCCFFG-UHFFFAOYSA-N
Formula:	C7H10
SMILES:	C=CC#CCCC
Mol. weight [g/mol]:	94.15
CAS:	2384-73-8

Physical Properties

Property code	Value	Unit	Source
gf	298.70	kJ/mol	Joback Method
hf	209.92	kJ/mol	Joback Method
hfus	15.73	kJ/mol	Joback Method
hvap	32.66	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	1.976		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	381.90 ± 2.00	K	NIST Webbook
tc	557.72	K	Joback Method
tf	272.99	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.30	J/mol×K	365.24	Joback Method
cpg	168.23	J/mol×K	397.32	Joback Method
cpg	177.73	J/mol×K	429.40	Joback Method
cpg	186.83	J/mol×K	461.48	Joback Method
cpg	195.52	J/mol×K	493.56	Joback Method
cpg	203.84	J/mol×K	525.64	Joback Method
cpg	211.78	J/mol×K	557.72	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54635e+01
Coeff. B	-3.62483e+03
Coeff. C	-4.76660e+01
Temperature range (K), min.	286.52
Temperature range (K), max.	404.72

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2384738&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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