

1,6-Heptadien-3-yne

Inchi:	InChI=1S/C7H8/c1-3-5-7-6-4-2/h3-4H,1-2,5H2
InchiKey:	PNMYNXREEKCUGV-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C=CC#CCC=C
Mol. weight [g/mol]:	92.14
CAS:	5150-80-1

Physical Properties

Property code	Value	Unit	Source
gf	386.54	kJ/mol	Joback Method
hf	335.35	kJ/mol	Joback Method
hfus	14.45	kJ/mol	Joback Method
hvap	31.99	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.752		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
tb	361.92	K	Joback Method
tc	558.76	K	Joback Method
tf	271.23	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.84	J/mol×K	361.92	Joback Method
cpg	154.05	J/mol×K	394.73	Joback Method
cpg	162.82	J/mol×K	427.53	Joback Method
cpg	171.15	J/mol×K	460.34	Joback Method
cpg	179.07	J/mol×K	493.15	Joback Method
cpg	186.59	J/mol×K	525.95	Joback Method
cpg	193.74	J/mol×K	558.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38554e+01
Coeff. B	-3.15931e+03
Coeff. C	-4.76660e+01
Temperature range (K), min.	280.52
Temperature range (K), max.	417.44

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=C5150801&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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