

1,7-Octadiyne

Other names:	octa-1,7-diyne
Inchi:	InChI=1S/C8H10/c1-3-5-7-8-6-4-2/h1-2H,5-8H2
InchiKey:	DSOJWVLXZNRKCS-UHFFFAOYSA-N
Formula:	C8H10
SMILES:	C#CCCCC#C
Mol. weight [g/mol]:	106.17
CAS:	871-84-1

Physical Properties

Property code	Value	Unit	Source
gf	462.62	kJ/mol	Joback Method
hf	375.35	kJ/mol	Joback Method
hfus	22.43	kJ/mol	Joback Method
hvap	33.12	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.813		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	769.20		NIST Webbook
tb	408.70	K	NIST Webbook
tb	409.00 ± 4.00	K	NIST Webbook
tb	408.50 ± 0.50	K	NIST Webbook
tc	550.52	K	Joback Method
tf	273.86	K	Joback Method
vc	0.407	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.80	J/mol×K	362.68	Joback Method
cpg	194.90	J/mol×K	393.99	Joback Method
cpg	204.49	J/mol×K	425.29	Joback Method
cpg	213.60	J/mol×K	456.60	Joback Method
cpg	222.24	J/mol×K	487.90	Joback Method

cpg	230.43	J/mol×K	519.21	Joback Method
cpg	238.21	J/mol×K	550.52	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63158e+01
Coeff. B	-4.13793e+03
Coeff. C	-5.47550e+01
Temperature range (K), min.	300.15
Temperature range (K), max.	430.78

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C871841&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/ci9903071
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

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

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