

1-Decen-3-yne

Inchi:	InChI=1S/C10H16/c1-3-5-7-9-10-8-6-4-2/h3H,1,4,6,8-10H2,2H3
InchiKey:	GGFFPUFVAVUWAN-UHFFFAOYSA-N
Formula:	C10H16
SMILES:	C=CC#CCCCCCC
Mol. weight [g/mol]:	136.23
CAS:	33622-26-3

Physical Properties

Property code	Value	Unit	Source
gf	323.96	kJ/mol	Joback Method
hf	148.00	kJ/mol	Joback Method
hfus	23.50	kJ/mol	Joback Method
hvap	39.34	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.146		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	348.20 ± 2.00	K	NIST Webbook
tc	622.23	K	Joback Method
tf	306.80	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.15	J/mol×K	433.88	Joback Method
cpg	286.02	J/mol×K	465.27	Joback Method
cpg	299.28	J/mol×K	496.66	Joback Method
cpg	311.96	J/mol×K	528.06	Joback Method
cpg	324.08	J/mol×K	559.45	Joback Method
cpg	335.66	J/mol×K	590.84	Joback Method
cpg	346.71	J/mol×K	622.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37931e+01
Coeff. B	-3.62628e+03
Coeff. C	-6.34560e+01
Temperature range (K), min.	331.96
Temperature range (K), max.	491.00

Sources

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=C33622263&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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