

1-Undecen-3-yne

Inchi:	InChI=1S/C11H18/c1-3-5-7-9-11-10-8-6-4-2/h3H,1,4,6,8-11H2,2H3
InchiKey:	GRUGRJDWWGWGPL-UHFFFAOYSA-N
Formula:	C11H18
SMILES:	C=CC#CCCCCCCC
Mol. weight [g/mol]:	150.26
CAS:	74744-28-8

Physical Properties

Property code	Value	Unit	Source
gf	332.38	kJ/mol	Joback Method
hf	127.36	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	41.56	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.536		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
tb	456.76	K	Joback Method
tc	643.32	K	Joback Method
tf	318.07	K	Joback Method
vc	0.595	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.59	J/mol×K	456.76	Joback Method
cpg	329.49	J/mol×K	487.85	Joback Method
cpg	343.75	J/mol×K	518.95	Joback Method
cpg	357.37	J/mol×K	550.04	Joback Method
cpg	370.40	J/mol×K	581.13	Joback Method
cpg	382.83	J/mol×K	612.22	Joback Method
cpg	394.70	J/mol×K	643.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48949e+01
Coeff. B	-4.18290e+03
Coeff. C	-7.29640e+01
Temperature range (K), min.	359.32
Temperature range (K), max.	509.43

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=C74744288&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

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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