

1,10-undecadiyne

Inchi:	InChI=1S/C11H16/c1-3-5-7-9-11-10-8-6-4-2/h1-2H,5-11H2
InchiKey:	PZWZXAPXSJTOOI-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	C#CCCCCCCC#C
Mol. weight [g/mol]:	148.24

Physical Properties

Property code	Value	Unit	Source
gf	487.88	kJ/mol	Joback Method
hf	313.43	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	39.80	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.984		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	431.32	K	Joback Method
tc	615.59	K	Joback Method
tf	307.67	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.99	J/molxK	431.32	Joback Method
cpg	312.77	J/molxK	462.03	Joback Method
cpg	325.89	J/molxK	492.74	Joback Method
cpg	338.37	J/molxK	523.45	Joback Method
cpg	350.25	J/molxK	554.17	Joback Method
cpg	361.56	J/molxK	584.88	Joback Method
cpg	372.31	J/molxK	615.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=T999919276&Units=SI
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

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

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