5-Undecen-3yne

Inchi: InChI=1S/C11H18/c1-3-5-7-9-11-10-8-6-4-2/h10-11H,3-5,7,9H2,1-2H3/b11-10+
InchiKey: HKGRHUQPBWLCLA-ZHACJKMWSA-N
Formula: C11H18
SMILES: CCC#CC=CCCCCC
Mol. weight [g/mol]: 150.26

Physical Properties

Property code	Value	Unit	Source
gf	324.76	kJ/mol	Joback Method
hf	119.15	kJ/mol	Joback Method
hfus	27.57	kJ/mol	Joback Method
hvap	42.19	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.536		Crippen Method
mcvol	152.950	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1161.00		NIST Webbook
ripol	1388.00		NIST Webbook
ripol	1388.00		NIST Webbook
tb	464.24	K	Joback Method
tc	655.79	K	Joback Method
tf	314.75	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.50	J/mol×K	464.24	Joback Method
cpg	330.70	J/mol×K	496.17	Joback Method
cpg	345.20	J/mol×K	528.09	Joback Method
cpg	359.01	J/mol×K	560.02	Joback Method
cpg	372.17	J/mol×K	591.94	Joback Method
cpg	384.70	J/mol×K	623.87	Joback Method

cpg	396.64	J/mol×K	655.79	Joback Method

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=R320291&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume