

1,11-Dodecadiyne

Inchi:	InChI=1S/C12H18/c1-3-5-7-9-11-12-10-8-6-4-2/h1-2H,5-12H2
InchiKey:	DVVJEEGECYXPEC-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	C#CCCCCCCCC#C
Mol. weight [g/mol]:	162.27
CAS:	20521-44-2

Physical Properties

Property code	Value	Unit	Source
gf	496.30	kJ/mol	Joback Method
hf	292.79	kJ/mol	Joback Method
hfus	32.79	kJ/mol	Joback Method
hvap	42.02	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.374		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	454.20	K	Joback Method
tc	636.86	K	Joback Method
tf	318.94	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.45	J/molxK	454.20	Joback Method
cpg	356.20	J/molxK	484.64	Joback Method
cpg	370.25	J/molxK	515.09	Joback Method
cpg	383.63	J/molxK	545.53	Joback Method
cpg	396.37	J/molxK	575.97	Joback Method
cpg	408.51	J/molxK	606.42	Joback Method
cpg	420.05	J/molxK	636.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.00	K	2.00	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20521442&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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