

3,9-Dodecadiyne

Inchi:	InChI=1S/C12H18/c1-3-5-7-9-11-12-10-8-6-4-2/h3-4,9-12H2,1-2H3
InchiKey:	SLQXYOMUNKJHRV-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCC#CCCCC#CCC
Mol. weight [g/mol]:	162.27
CAS:	61827-89-2

Physical Properties

Property code	Value	Unit	Source
gf	455.76	kJ/mol	Joback Method
hf	253.59	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.374		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	491.96	K	Joback Method
tc	696.84	K	Joback Method
tf	437.20	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.46	J/mol×K	491.96	Joback Method
cpg	361.21	J/mol×K	526.11	Joback Method
cpg	376.24	J/mol×K	560.25	Joback Method
cpg	390.60	J/mol×K	594.40	Joback Method
cpg	404.28	J/mol×K	628.55	Joback Method
cpg	417.33	J/mol×K	662.70	Joback Method
cpg	429.75	J/mol×K	696.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	329.60	K	0.07	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.37370e+01
Coeff. B	-3.98550e+03
Coeff. C	-7.50810e+01
Temperature range (K), min.	371.41
Temperature range (K), max.	548.10

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=C61827892&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/ci990307I
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/40-134-8/3-9-Dodecadiyne.pdf>

Generated by Cheméo on 2025-12-05 13:56:10.177560654 +0000 UTC m=+4691167.707601308.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.