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#CCCCCC#CCC
Mol. weight [g/mol]: 162.28
CAS: 61827-89-2

Physical Properties

Property code	Value	Unit	Source
af	0.3461		Cheméo Relay (1.0)
hf	181.80	kJ/mol	Cheméo Relay (1.0)
hfus	33.08	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-3.94		Cheméo Relay (1.0)
logp	3.374		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	465.75	K	Cheméo Relay (1.0)
tc	679.45	K	Cheméo Relay (1.0)
tf	242.09	K	Cheméo Relay (1.0)
vc	0.594	m3/kmol	Cheméo Relay (1.0)

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(Pvp) = 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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C61827892&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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