1-Dodecyne

Other names: 1-C12H22
dodec-1-yne
Inchi: InChI=1S/C12H22/c1-3-5-7-9-11-12-10-8-6-4-2/h1H,4-12H2,2H3
InchiKey: ZVDBUOGYYYNMQI-UHFFFAOYSA-N
Formula: C12H22
SMILES: C#CCCCCCCCCC
Mol. weight [g/mol]: 166.30
CAS: 765-03-7

Physical Properties

Property code	Value	Unit	Source
af	0.5120		KDB
gf	273.23	kJ/mol	Joback Method
hf	0.89	kJ/mol	Joback Method
hfus	29.81	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
ie	9.90 ± 0.02	eV	NIST Webbook
log10ws	-4.64		Crippen Method
logp	4.150		Crippen Method
mcvol	171.340	ml/mol	McGowan Method
pc	2030.00	kPa	KDB
rinpol	1213.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1197.00		NIST Webbook
rinpol	1185.00		NIST Webbook
ripol	1416.40		NIST Webbook
ripol	1432.00		NIST Webbook
ripol	1433.00		NIST Webbook
ripol	1404.80		NIST Webbook
ripol	1407.40		NIST Webbook
ripol	1427.80		NIST Webbook

ripol	1409.60		NIST Webbook
ripol	1428.90		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1410.30		NIST Webbook
ripol	1421.80		NIST Webbook
ripol	1433.00		NIST Webbook
tb	488.20	K	KDB
tb	488.00	K	NIST Webbook
tb	488.20	K	NIST Webbook
tc	668.20	K	KDB
tf	254.00	K	KDB
vc	0.669	m3/kmol	KDB
zc	0.2446260		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.41	J/mol×K	464.08	Joback Method
cpg	389.24	J/mol×K	492.60	Joback Method
cpg	404.41	J/mol×K	521.12	Joback Method
cpg	418.95	J/mol×K	549.64	Joback Method
cpg	432.87	J/mol×K	578.16	Joback Method
cpg	446.20	J/mol×K	606.68	Joback Method
cpg	458.96	J/mol×K	635.20	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.00	K	1.30	NIST Webbook

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46575e+01
Coeff. B	-4.24108e+03
Coeff. C	-6.55460e+01
Temperature range (K), min.	360.68
Temperature range (K), max.	519.33

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.15770e+01
Coeff. B	-8.49994e+03
Coeff. C	-6.44883e+00
Coeff. D	1.55993e-06
Temperature range (K), min.	386.15
Temperature range (K), max.	668.16

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol438.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C765037&Units=SI

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

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=438

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

af: Acentric Factor

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

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

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