1-Decyne

Other names: 1-C10H18
OCTYLACETYLENE
dec-1-yne
Inchi: InChI=1S/C10H18/c1-3-5-7-9-10-8-6-4-2/h1H,4-10H2,2H3
InchiKey: ILLHQJIJCRNRCJ-UHFFFAOYSA-N
Formula: C10H18
SMILES: C#CCCCCCCCC
Mol. weight [g/mol]: 138.25
CAS: 764-93-2

Physical Properties

Property code	Value	Unit	Source
af	0.4260		KDB
gf	256.39	kJ/mol	Joback Method
hf	41.90 ± 3.40	kJ/mol	NIST Webbook
hfus	24.63	kJ/mol	Joback Method
hvap	37.71	kJ/mol	Joback Method
ie	9.91 ± 0.02	eV	NIST Webbook
log10ws	-3.80		Crippen Method
logp	3.370		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2430.00	kPa	KDB
rinpol	983.00		NIST Webbook
rinpol	988.60		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1014.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	987.90		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	997.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	987.90		NIST Webbook

rinpol	984.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1211.10		NIST Webbook
ripol	1212.10		NIST Webbook
ripol	1230.00		NIST Webbook
ripol	1215.60		NIST Webbook
ripol	1221.90		NIST Webbook
ripol	1226.30		NIST Webbook
ripol	1234.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1233.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1235.00		NIST Webbook
ripol	1226.80		NIST Webbook
ripol	1228.80		NIST Webbook
tb	447.60	K	NIST Webbook
tb	447.20	K	NIST Webbook
tb	447.20	K	KDB
tc	632.50	K	KDB
tf	229.00	K	KDB
vc	0.557	m3/kmol	KDB
zc	0.2576050		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.22	J/mol×K	418.32	Joback Method
cpg	300.21	J/mol×K	447.22	Joback Method
cpg	313.62	J/mol×K	476.11	Joback Method
cpg	326.47	J/mol×K	505.01	Joback Method
cpg	338.77	J/mol×K	533.91	Joback Method
cpg	350.56	J/mol×K	562.80	Joback Method
cpg	361.83	J/mol×K	591.70	Joback Method
rfi	1.42490		298.15	KDB

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49423e+01
Coeff. B	-4.08278e+03
Coeff. C	-5.21330e+01
Temperature range (K), min.	330.73
Temperature range (K), max.	476.06

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.04556e+01
Coeff. B	-8.14464e+03
Coeff. C	-7.89639e+00
Coeff. D	2.85018e-06
Temperature range (K), min.	351.15
Temperature range (K), max.	632.49

Sources

Activity coefficients at infinite dilution of organic solutes in the ionic liquid trihexyltetradecylphosphonium hexafluorophosphate using gas liquid chromatography at T = (313.15, 333.15, 353.15, and 363.15) K:	https://www.doi.org/10.1016/j.jct.2012.01.004
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=435
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C764932&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent:	https://www.doi.org/10.1016/j.fluid.2006.07.015
Activity coefficients at infinite dilution for solutes in the trihexyltetradecylammonium bis(trifluoromethylsulfonyl)imide ionic liquid using gas liquid chromatography:	https://www.doi.org/10.1016/j.jct.2009.08.012
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol435.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rfi:	Refractive Index
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
zc:	Critical Compressibility