2-Decyne

Other names: 2-C10H18
Inchi: InChI=1S/C10H18/c1-3-5-7-9-10-8-6-4-2/h3,5,7-10H2,1-2H3
InchiKey: RWDDSTHSVISBEA-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC#CCCCCCCC
Mol. weight [g/mol]: 138.25
CAS: 2384-70-5

Physical Properties

Property code	Value	Unit	Source
gf	236.12	kJ/mol	Joback Method
hf	23.60 ± 3.40	kJ/mol	NIST Webbook
hfus	24.78	kJ/mol	Joback Method
hvap	40.01	kJ/mol	Joback Method
ie	9.30 ± 0.02	eV	NIST Webbook
log10ws	-3.80		Crippen Method
logp	3.370		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1041.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1051.00		NIST Webbook
rinpol	1041.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1041.00		NIST Webbook
ripol	1255.50		NIST Webbook
ripol	1256.90		NIST Webbook
ripol	1251.70		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1264.00		NIST Webbook

ripol	1265.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1234.50		NIST Webbook
ripol	1253.20		NIST Webbook
ripol	1237.10		NIST Webbook
ripol	1240.70		NIST Webbook
ripol	1248.00		NIST Webbook
tb	437.20	K	Joback Method
tc	621.64	K	Joback Method
tf	308.56	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.31	J/mol×K	437.20	Joback Method
cpg	302.76	J/mol×K	467.94	Joback Method
cpg	316.63	J/mol×K	498.68	Joback Method
cpg	329.93	J/mol×K	529.42	Joback Method
cpg	342.68	J/mol×K	560.16	Joback Method
cpg	354.90	J/mol×K	590.90	Joback Method
cpg	366.61	J/mol×K	621.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.00	K	3.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54033e+01
Coeff. B	-4.19906e+03

Coeff. C	-6.84040e+01
Temperature range (K), min.	346.20
Temperature range (K), max.	484.49

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol436.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2384705&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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

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