4,6-Decadiyne

Inchi: InChI=1S/C10H14/c1-3-5-7-9-10-8-6-4-2/h3-6H2,1-2H3
InchiKey: LIWZSNTUMSGWTF-UHFFFAOYSA-N
Formula: C10H14
SMILES: CCCC#CC#CCCC
Mol. weight [g/mol]: 134.22
CAS: 16387-71-6

Physical Properties

Property code	Value	Unit	Source
gf	438.92	kJ/mol	Joback Method
hf	294.87	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	42.16	kJ/mol	Joback Method
ie	8.72	eV	NIST Webbook
log10ws	-3.60		Crippen Method
logp	2.593		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	446.20	K	Joback Method
tc	656.77	K	Joback Method
tf	414.66	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.80	J/mol×K	446.20	Joback Method
cpg	273.31	J/mol×K	481.29	Joback Method
cpg	286.24	J/mol×K	516.39	Joback Method
cpg	298.58	J/mol×K	551.48	Joback Method
cpg	310.37	J/mol×K	586.58	Joback Method
cpg	321.61	J/mol×K	621.67	Joback Method
cpg	332.33	J/mol×K	656.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.00	K	0.30	NIST Webbook
tbrp	361.00	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49481e+01
Coeff. B	-4.15561e+03
Coeff. C	-6.82230e+01
Temperature range (K), min.	351.68
Temperature range (K), max.	499.45

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16387716&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

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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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