1,9-Decadiyne

Other names: deca-1,9-diyne
Inchi: InChI=1S/C10H14/c1-3-5-7-9-10-8-6-4-2/h1-2H,5-10H2
InchiKey: ILVDYAGPHFWNQI-UHFFFAOYSA-N
Formula: C10H14
SMILES: C#CCCCCCCC#C
Mol. weight [g/mol]: 134.22
CAS: 1720-38-3

Physical Properties

Property code	Value	Unit	Source
gf	479.46	kJ/mol	Joback Method
hf	334.07	kJ/mol	Joback Method
hfus	27.61	kJ/mol	Joback Method
hvap	37.57	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.593		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	408.44	K	Joback Method
tc	594.16	K	Joback Method
tf	296.40	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.65	J/mol×K	408.44	Joback Method
cpg	271.33	J/mol×K	439.39	Joback Method
cpg	283.40	J/mol×K	470.35	Joback Method
cpg	294.88	J/mol×K	501.30	Joback Method
cpg	305.80	J/mol×K	532.25	Joback Method
cpg	316.18	J/mol×K	563.21	Joback Method
cpg	326.04	J/mol×K	594.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.00 ± 1.00	K	1.70	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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1720383&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

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
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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