3-Octyne, 7-methyl-

Other names: 7-Methyl-3-octyne
Inchi: InChI=1S/C9H16/c1-4-5-6-7-8-9(2)3/h9H,4,7-8H2,1-3H3
InchiKey: ZDXUMWBWHSCWBK-UHFFFAOYSA-N
Formula: C9H16
SMILES: CCC#CCCC(C)C
Mol. weight [g/mol]: 124.22
CAS: 37050-06-9

Physical Properties

Property code	Value	Unit	Source
gf	225.26	kJ/mol	Joback Method
hf	37.93	kJ/mol	Joback Method
hfus	18.67	kJ/mol	Joback Method
hvap	37.39	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.836		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	413.88	K	Joback Method
tc	604.24	K	Joback Method
tf	282.29	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.21	J/mol×K	413.88	Joback Method
cpg	260.92	J/mol×K	445.61	Joback Method
cpg	274.08	J/mol×K	477.33	Joback Method
cpg	286.69	J/mol×K	509.06	Joback Method
cpg	298.77	J/mol×K	540.78	Joback Method
cpg	310.34	J/mol×K	572.51	Joback Method
cpg	321.40	J/mol×K	604.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.00	K	13.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52610e+01
Coeff. B	-3.88910e+03
Coeff. C	-5.87860e+01
Temperature range (K), min.	318.52
Temperature range (K), max.	449.67

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37050069&Units=SI

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

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