7-Methyl-1-nonyne

Other names: 7-Methyl-non-1-yne
Inchi: InChI=1S/C10H18/c1-4-6-7-8-9-10(3)5-2/h1,10H,5-9H2,2-3H3
InchiKey: ILTCNNWNFZMWTJ-UHFFFAOYSA-N
Formula: C10H18
SMILES: C#CCCCCC(C)CC
Mol. weight [g/mol]: 138.25
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.3683		Cheméo Relay (1.0)
gf	253.95	kJ/mol	Joback Method
hf	4.09	kJ/mol	Cheméo Relay (1.0)
hfus	21.11	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-4.61		Cheméo Relay (1.0)
logp	3.226		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
tb	439.57	K	Cheméo Relay (1.0)
tc	619.22	K	Cheméo Relay (1.0)
tf	198.16	K	Cheméo Relay (1.0)
vc	0.499	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.20	J/mol×K	417.88	Joback Method
cpg	300.59	J/mol×K	447.43	Joback Method
cpg	314.37	J/mol×K	476.99	Joback Method
cpg	327.56	J/mol×K	506.54	Joback Method
cpg	340.18	J/mol×K	536.09	Joback Method
cpg	352.24	J/mol×K	565.64	Joback Method

cpg	363.76	J/mol×K	595.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50342e+01
Coeff. B	-3.98416e+03
Coeff. C	-6.43460e+01
Temperature range (K), min.	334.52
Temperature range (K), max.	474.12

Sources

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C71566659&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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