3-Octyne, 2,2-dimethyl-

Other names: 2,2-Dimethyl-3-octyne
Inchi: InChI=1S/C10H18/c1-5-6-7-8-9-10(2,3)4/h5-7H2,1-4H3
InchiKey: XBLMXBDWMYMTLK-UHFFFAOYSA-N
Formula: C10H18
SMILES: CCCCC#CC(C)(C)C
Mol. weight [g/mol]: 138.25
CAS: 19482-57-6

Physical Properties

Property code	Value	Unit	Source
gf	238.96	kJ/mol	Joback Method
hf	13.82	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	38.71	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.226		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	433.97	K	Joback Method
tc	630.64	K	Joback Method
tf	310.98	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.42	J/mol×K	433.97	Joback Method
cpg	306.36	J/mol×K	466.75	Joback Method
cpg	321.48	J/mol×K	499.53	Joback Method
cpg	335.83	J/mol×K	532.31	Joback Method
cpg	349.43	J/mol×K	565.08	Joback Method
cpg	362.32	J/mol×K	597.86	Joback Method
cpg	374.53	J/mol×K	630.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44054e+01
Coeff. B	-3.76269e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	328.92
Temperature range (K), max.	476.16

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=C19482576&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
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume