2-Methyl-1-nonene-3-yne

Other names: 2-Methyl-1-nonen-3-yne
1-Nonen-3-yne, 2-methyl-
Inchi: InChI=1S/C10H16/c1-4-5-6-7-8-9-10(2)3/h2,4-7H2,1,3H3
InchiKey: GSFPEKGMYODGNK-UHFFFAOYSA-N
Formula: C10H16
SMILES: C=C(C)C#CCCCCC
Mol. weight [g/mol]: 136.23
CAS: 70058-00-3

Physical Properties

Property code	Value	Unit	Source
gf	315.41	kJ/mol	Joback Method
hf	138.21	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	39.42	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.146		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	433.76	K	Joback Method
tc	625.81	K	Joback Method
tf	292.84	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.09	J/mol×K	433.76	Joback Method
cpg	286.19	J/mol×K	465.77	Joback Method
cpg	299.66	J/mol×K	497.78	Joback Method
cpg	312.54	J/mol×K	529.79	Joback Method
cpg	324.82	J/mol×K	561.80	Joback Method
cpg	336.55	J/mol×K	593.80	Joback Method
cpg	347.73	J/mol×K	625.81	Joback Method

Sources

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=C70058003&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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