

3-Octyne, 2-methyl-

Inchi:	InChI=1S/C9H16/c1-4-5-6-7-8-9(2)3/h9H,4-6H2,1-3H3
InchiKey:	VGZZDWCLCYQULT-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CCCCC#CC(C)C
Mol. weight [g/mol]:	124.22
CAS:	55402-15-8

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	417.00 ± 5.00	K	NIST Webbook
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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55402158&Units=SI
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

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

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