(E)-5-Methyl-3-hexen-1-yne

Inchi: InChI=1S/C7H10/c1-4-5-6-7(2)3/h1,5-7H,2-3H3/b6-5+
InchiKey: YPAAIRQADKROCE-AATRIKPKSA-N
Formula: C7H10
SMILES: C#CC=CC(C)C
Mol. weight [g/mol]: 94.15
CAS: 80033-69-8

Physical Properties

Property code	Value	Unit	Source
gf	308.91	kJ/mol	Joback Method
hf	216.03	kJ/mol	Joback Method
hfus	13.54	kJ/mol	Joback Method
hvap	30.60	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.832		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	353.40	K	Joback Method
tc	543.00	K	Joback Method
tf	195.54	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.90	J/mol×K	353.40	Joback Method
cpg	168.40	J/mol×K	385.00	Joback Method
cpg	178.33	J/mol×K	416.60	Joback Method
cpg	187.73	J/mol×K	448.20	Joback Method
cpg	196.62	J/mol×K	479.80	Joback Method
cpg	205.03	J/mol×K	511.40	Joback Method
cpg	212.98	J/mol×K	543.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80033698&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