(E)-5,5-Dimethyl-3-hexen-1-yne

Inchi: InChI=1S/C8H12/c1-5-6-7-8(2,3)4/h1,6-7H,2-4H3/b7-6+
InchiKey: HTRVREURCYRGAX-VOTSOKGWSA-N
Formula: C8H12
SMILES: C#CC=CC(C)(C)C
Mol. weight [g/mol]: 108.18
CAS: 80033-71-2

Physical Properties

Property code	Value	Unit	Source
gf	322.61	kJ/mol	Joback Method
hf	191.92	kJ/mol	Joback Method
hfus	12.24	kJ/mol	Joback Method
hvap	31.92	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.222		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	373.49	K	Joback Method
tc	570.74	K	Joback Method
tf	224.23	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.49	J/mol×K	373.49	Joback Method
cpg	207.64	J/mol×K	406.36	Joback Method
cpg	219.94	J/mol×K	439.24	Joback Method
cpg	231.44	J/mol×K	472.11	Joback Method
cpg	242.18	J/mol×K	504.99	Joback Method
cpg	252.22	J/mol×K	537.86	Joback Method
cpg	261.60	J/mol×K	570.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80033712&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