4-octyne, 2,7-dimethyl

Inchi: InChI=1S/C10H18/c1-9(2)7-5-6-8-10(3)4/h9-10H,7-8H2,1-4H3
InchiKey: KCLRHUYFDJVIFV-UHFFFAOYSA-N
Formula: C10H18
SMILES: CC(C)CC#CCC(C)C
Mol. weight [g/mol]: 138.25

Physical Properties

Property code	Value	Unit	Source
gf	231.24	kJ/mol	Joback Method
hf	12.01	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	39.23	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.082		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	930.00		NIST Webbook
tb	436.32	K	Joback Method
tc	629.38	K	Joback Method
tf	278.56	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.39	J/mol×K	436.32	Joback Method
cpg	303.69	J/mol×K	468.50	Joback Method
cpg	318.34	J/mol×K	500.67	Joback Method
cpg	332.36	J/mol×K	532.85	Joback Method
cpg	345.76	J/mol×K	565.03	Joback Method
cpg	358.56	J/mol×K	597.20	Joback Method
cpg	370.78	J/mol×K	629.38	Joback Method

Sources

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=R66700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume