1-Octen-4-yne

Inchi: InChI=1S/C8H12/c1-3-5-7-8-6-4-2/h3H,1,4-6H2,2H3
InchiKey: ICBXOVYWGIDVQO-UHFFFAOYSA-N
Formula: C8H12
SMILES: C=CCC#CCCC
Mol. weight [g/mol]: 108.18
CAS: 24612-83-7

Physical Properties

Property code	Value	Unit	Source
gf	307.12	kJ/mol	Joback Method
hf	189.28	kJ/mol	Joback Method
hfus	18.32	kJ/mol	Joback Method
hvap	34.88	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3142.03	kPa	Joback Method
tb	388.12	K	Joback Method
tc	579.51	K	Joback Method
tf	284.26	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.89	J/mol×K	388.12	Joback Method
cpg	205.28	J/mol×K	420.02	Joback Method
cpg	216.17	J/mol×K	451.92	Joback Method
cpg	226.59	J/mol×K	483.82	Joback Method
cpg	236.55	J/mol×K	515.72	Joback Method
cpg	246.07	J/mol×K	547.61	Joback Method
cpg	255.16	J/mol×K	579.51	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=C24612837&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