1,4-Octadiyne

Inchi: InChI=1S/C8H10/c1-3-5-7-8-6-4-2/h1H,4-6H2,2H3
InchiKey: CQOOLRZHDLXBJM-UHFFFAOYSA-N
Formula: C8H10
SMILES: C#CCC#CCCC
Mol. weight [g/mol]: 106.17

Physical Properties

Property code	Value	Unit	Source
gf	442.35	kJ/mol	Joback Method
hf	355.75	kJ/mol	Joback Method
hfus	22.57	kJ/mol	Joback Method
hvap	35.41	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.813		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	811.80		NIST Webbook
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tb	381.56	K	Joback Method
tc	583.07	K	Joback Method
tf	332.99	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.04	J/mol×K	381.56	Joback Method
cpg	194.38	J/mol×K	415.15	Joback Method
cpg	204.23	J/mol×K	448.73	Joback Method
cpg	213.62	J/mol×K	482.32	Joback Method
cpg	222.57	J/mol×K	515.90	Joback Method
cpg	231.08	J/mol×K	549.49	Joback Method
cpg	239.19	J/mol×K	583.07	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=R144795&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume