

2,2,5,5,8,8-Hexamethylnona-3,6-diyne

Inchi:	InChI=1S/C15H24/c1-13(2,3)9-11-15(7,8)12-10-14(4,5)6/h1-8H3
InchiKey:	XQCLEAPKEXXCOD-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CC(C)(C)C#CC(C)(C)C#CC(C)(C)C
Mol. weight [g/mol]:	204.35
CAS:	116503-39-0

Physical Properties

Property code	Value	Unit	Source
gf	489.54	kJ/mol	Joback Method
hf	165.42	kJ/mol	Joback Method
hfus	18.61	kJ/mol	Joback Method
hvap	49.40	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.112		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
tb	550.91	K	Joback Method
tc	786.88	K	Joback Method
tf	478.27	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	497.12	J/molxK	550.91	Joback Method
cpg	519.07	J/molxK	590.24	Joback Method
cpg	539.40	J/molxK	629.57	Joback Method
cpg	558.26	J/molxK	668.90	Joback Method
cpg	575.76	J/molxK	708.23	Joback Method
cpg	592.02	J/molxK	747.56	Joback Method
cpg	607.18	J/molxK	786.88	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=C116503390&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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