3-Octen-5-yne, 2,2,7,7-tetramethyl-

Other names: 2,2,7,7-Tetramethyl-3-octen-5-yne
Inchi: InChI=1S/C12H20/c1-11(2,3)9-7-8-10-12(4,5)6/h7,9H,1-6H3/b9-7+
InchiKey: SJKGMWBQDQMRKQ-VQHVLOKHSA-N
Formula: C12H20
SMILES: CC(C)(C)C#CC=CC(C)(C)C
Mol. weight [g/mol]: 164.29
CAS: 55682-74-1

Physical Properties

Property code	Value	Unit	Source
gf	338.86	kJ/mol	Joback Method
hf	81.01	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.638		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
tb	480.66	K	Joback Method
tc	695.61	K	Joback Method
tf	330.86	K	Joback Method
vc	0.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.53	J/mol×K	480.66	Joback Method
cpg	384.49	J/mol×K	516.48	Joback Method
cpg	402.18	J/mol×K	552.31	Joback Method
cpg	418.68	J/mol×K	588.13	Joback Method
cpg	434.07	J/mol×K	623.96	Joback Method
cpg	448.43	J/mol×K	659.78	Joback Method
cpg	461.85	J/mol×K	695.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55682741&Units=SI

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