3-Heptyne, 2,2,6,6-tetramethyl

Inchi: InChI=1S/C11H20/c1-10(2,3)8-7-9-11(4,5)6/h8H2,1-6H3
InchiKey: MJLMFLNLBQSVFD-UHFFFAOYSA-N
Formula: C11H20
SMILES: CC(C)(C)C#CCC(C)(C)C
Mol. weight [g/mol]: 152.28

Physical Properties

Property code	Value	Unit	Source
gf	250.22	kJ/mol	Joback Method
hf	-15.57	kJ/mol	Joback Method
hfus	12.54	kJ/mol	Joback Method
hvap	39.64	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.472		Crippen Method
mcvol	157.250	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	857.00		NIST Webbook
tb	453.62	K	Joback Method
tc	661.20	K	Joback Method
tf	324.67	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.14	J/mol×K	453.62	Joback Method
cpg	354.62	J/mol×K	488.22	Joback Method
cpg	371.97	J/mol×K	522.81	Joback Method
cpg	388.26	J/mol×K	557.41	Joback Method
cpg	403.54	J/mol×K	592.01	Joback Method
cpg	417.87	J/mol×K	626.61	Joback Method
cpg	431.31	J/mol×K	661.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R66625&Units=SI
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

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

Latest version available from:

https://www.chemeo.com/cid/74-400-5/3-Heptyne-2-2-6-6-tetramethyl.pdf

Generated by Cheméo on 2024-10-12 07:58:23.032809007 +0000 UTC m=+3300765.669778255.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.